

=> d his ful

FILE 'REGISTRY' ENTERED AT 15:23:58 ON 23 NOV 2007

L132 STR
L133 25 SEA SSS SAM L132
L134 383 SEA SSS FUL L132
L135 STR
L136 26 SEA SUB=L134 SSS FUL L135

FILE 'HCAPLUS' ENTERED AT 15:31:41 ON 23 NOV 2007

L137 3 SEA ABB=ON PLU=ON L136
D STAT QUE L137
D IBIB ABS HITSTR L137 1-3
L138 292 SEA ABB=ON PLU=ON "CHUNG SUNG"/AU OR "CHUNG SUNG KEE"/AU OR
CHUNG S/AU OR CHUNG S K?/AU
L139 5 SEA ABB=ON PLU=ON "JEON O Y"/AU OR ("JEON OCK YOUM"/AU OR
"JEON OCK YOUNM"/AU)
L140 1574 SEA ABB=ON PLU=ON KUMAR K/AU OR KUMAR K ?/AU
L141 540 SEA ABB=ON PLU=ON "YU SEOK"/AU OR "YU SEOK HO"/AU OR YU S/AU
OR YU S H?/AU
L142 16 SEA ABB=ON PLU=ON L138 AND (L139 OR L140 OR L141)
L143 2 SEA ABB=ON PLU=ON L139 AND (L140 OR L141)
L144 0 SEA ABB=ON PLU=ON L140 AND L141

FILE 'REGISTRY' ENTERED AT 15:38:19 ON 23 NOV 2007

L145 357 SEA ABB=ON PLU=ON L134 NOT L136

FILE 'HCAPLUS' ENTERED AT 15:38:24 ON 23 NOV 2007

L146 720 SEA ABB=ON PLU=ON L145
L147 1 SEA ABB=ON PLU=ON (L138 OR L139 OR L140 OR L141) AND L146
L148 13 SEA ABB=ON PLU=ON (L142 OR L143 OR L144 OR L147) NOT L137
D STAT QUE L148
D IBIB ABS HITSTR L148 1-13

FILE 'REGISTRY' ENTERED AT 15:40:58 ON 23 NOV 2007

L149 STR
L151 5 SEA SSS FUL L149

FILE 'HCAPLUS' ENTERED AT 15:43:07 ON 23 NOV 2007

L152 2 SEA ABB=ON PLU=ON L151
D STAT QUE L152
D IBIB ABS HITSTR L152 1-2

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 22 NOV 2007 HIGHEST RN 955628-80-5

DICTIONARY FILE UPDATES: 22 NOV 2007 HIGHEST RN 955628-80-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

FILE HCAPLUS

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FILE COVERS 1907 - 23 Nov 2007 VOL 147 ISS 23
FILE LAST UPDATED: 22 Nov 2007 (20071122/ED)

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New CAS Information Use Policies, enter HELP USAGETERMS for details.

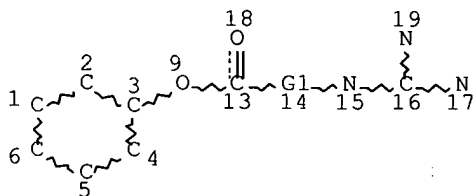
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DEFAULT ECLEVEL IS LIMITED

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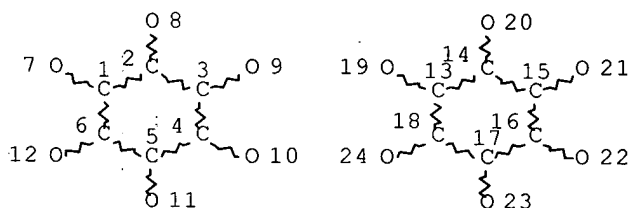
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NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L134 383 SEA FILE=REGISTRY SSS FUL L132

L135 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

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NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

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L137 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L136

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=> d ibib abs hitstr l137 1-3

L137 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2007:107441 HCAPLUS Full-text

DOCUMENT NUMBER: 146:359080

TITLE: Design, synthesis, and delivery properties of novel

POST PRIORITY & FILING

guanidine-containing molecular transporters built on dimeric inositol scaffolds

AUTHOR(S): Maiti, Kaustabh K.; Jeon, Ock-Youm; Lee, Woo Sirl; Chung, Sung-Kee

CORPORATE SOURCE: Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science & Technology, Pohang, 790-784, S. Korea

SOURCE: Chemistry--A European Journal (2007), 13(3), 762-775
CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We have developed a novel class of synthetic mol. transporters that contain eight residues of guanidine with an inositol dimer as the scaffold. The dimers were prepared by connecting two units of myo- or scyllo-inositol via a carbonate or amide linkage, and the multiple units of the guanidine functionality were constructed on the inositol scaffold by means of per-acylation with ω -aminocarboxylate derivs. of varying length. Bioassays based on confocal laser scanning microscopy and fluorescence-activated cell sorter analyses indicated that these transporters display a varying degree of membrane translocating ability, and the intracellular localization and mouse-tissue distribution studies strongly suggested that these transporters undergo substantially different mechanistic processes from those of peptide transporters reported to date. It was also shown that doxorubicin, an anticancer antibiotic, can be efficiently delivered into mouse brain by aid of this type of transporter.

IT 898815-49-1P 898815-54-8P 898815-81-1P
929623-34-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

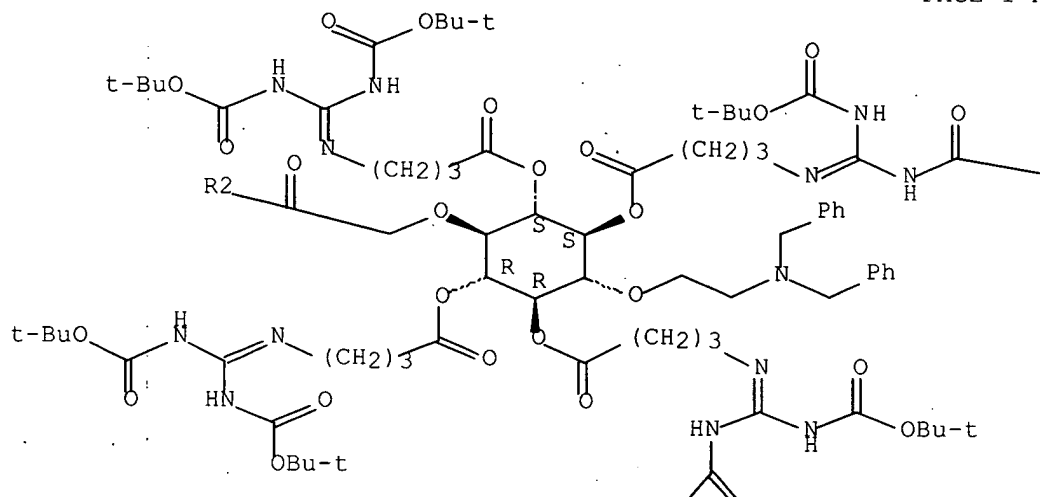
(design, synthesis, and delivery properties of novel guanidine-containing mol. transporters built on dimeric inositol scaffolds)

RN 898815-49-1 HCAPLUS

CN scyllo-Inositol, 1-O-[2-[bis(phenylmethyl)amino]ethyl]-4-O-[2-[[2-[2,3,5,6-tetrakis-O-[4-[[bis[[[(1,1-dimethylethoxy)carbonyl]amino]methylene]amino]-1-oxobutyl]-4-O-(2-methoxy-2-oxoethyl)-scyllo-inositol-1-O-yl]ethyl]amino]-2-oxoethyl]-, 2,3,5,6-tetrakis[4-[[bis[[[(1,1-dimethylethoxy)carbonyl]amino]methylene]amino]butanoate] (CA INDEX NAME)

Relative stereochemistry.

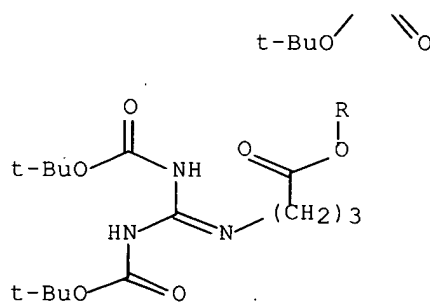
PAGE 1-A



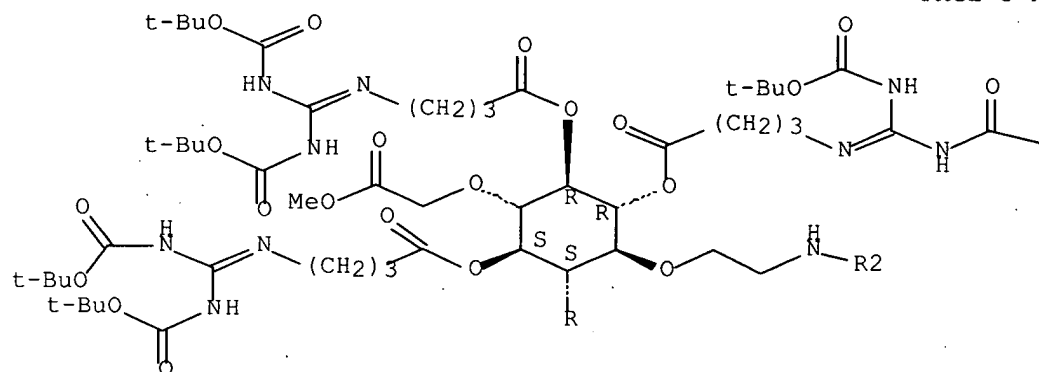
PAGE 1-B

—OBu-t

PAGE 2-A



PAGE 3-A



PAGE 3-B

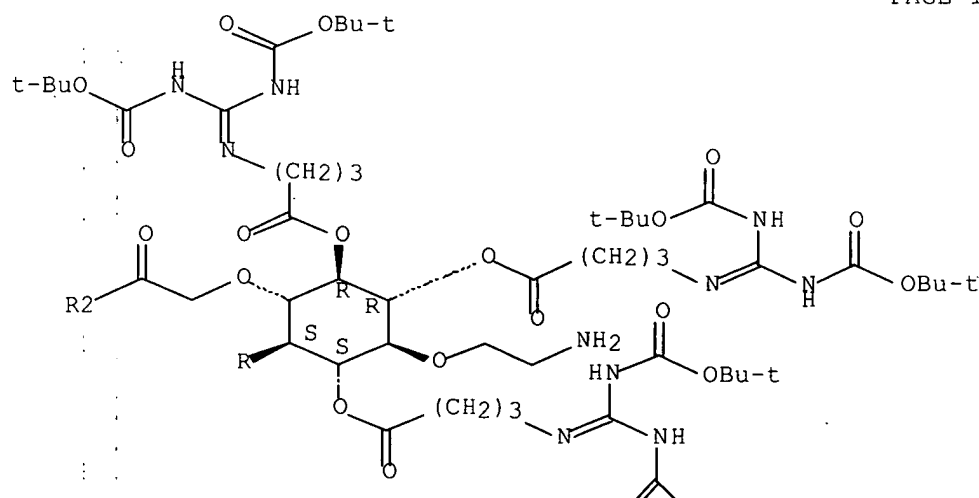
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RN 898815-54-8 HCAPLUS

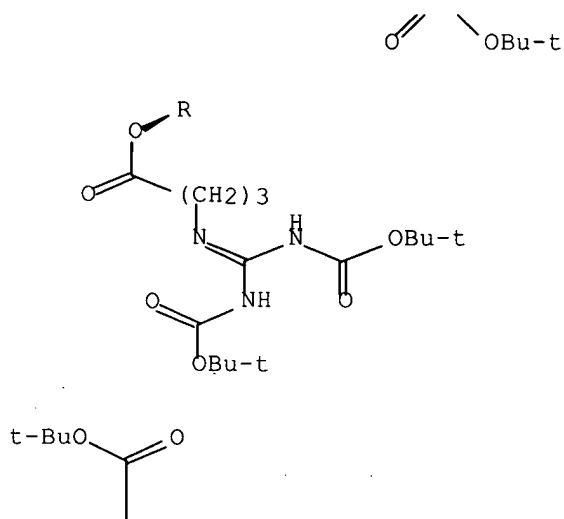
CN scyllo-Inositol, 1-O-[2-[[[4-O-(2-aminoethyl)-2,3,5,6-tetrakis-O-[4-
[[bis[[(1,1-dimethylethoxy)carbonyl]amino]methylene]amino]-1-oxobutyl]-
scyllo-inositol-1-O-yl]acetyl]amino]ethyl]-4-O-(2-methoxy-2-oxoethyl)-,
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no]butanoate] (CA INDEX NAME)

Relative stereochemistry.

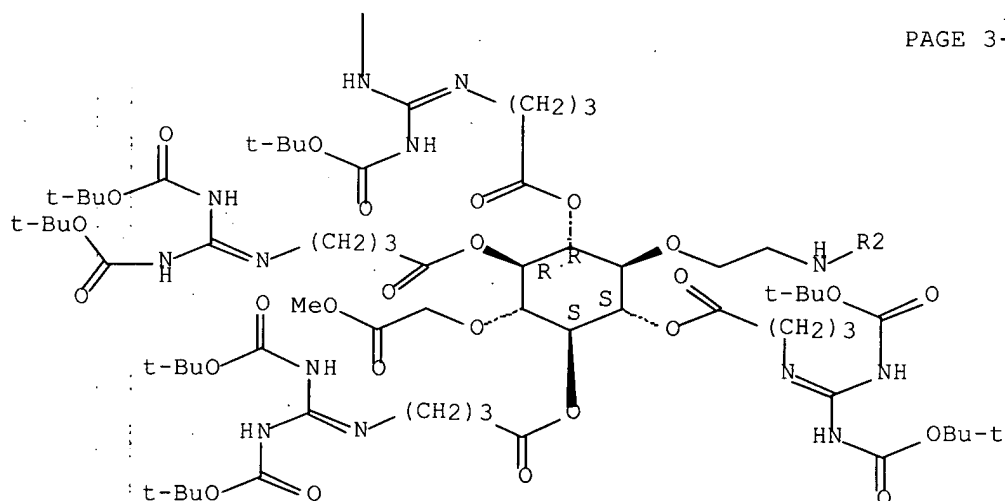
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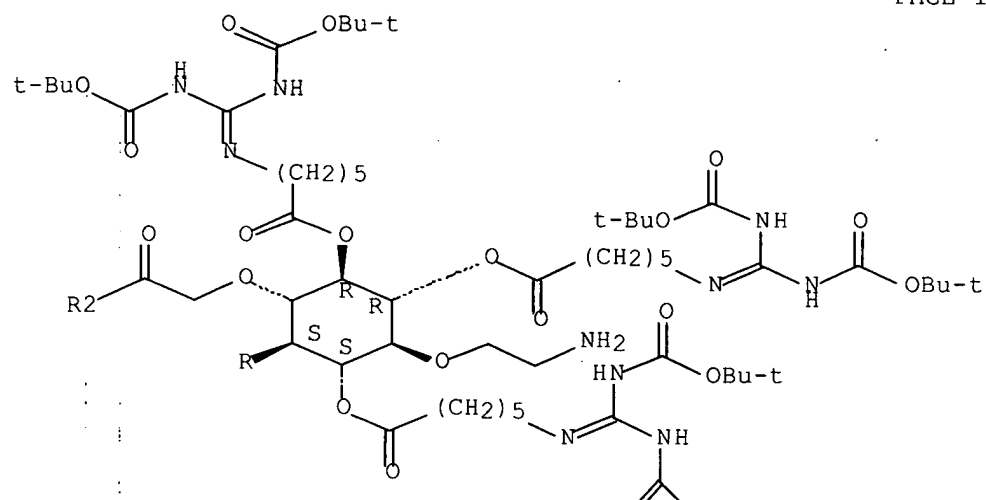
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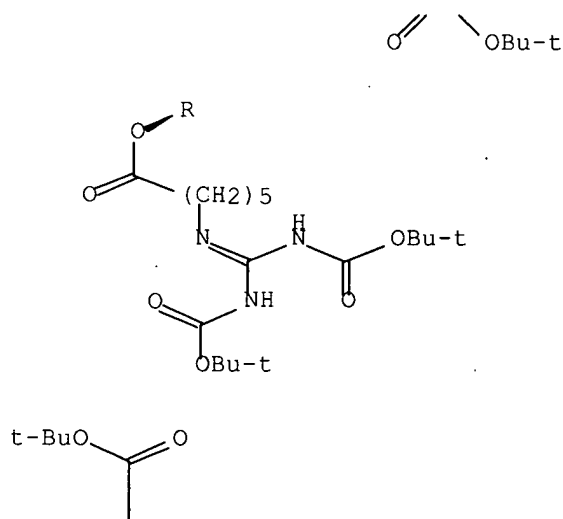
RN 898815-81-1 HCAPLUS
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 [[bis[[(1,1-dimethylethoxy)carbonyl]amino]methylene]amino]-1-oxohexyl]-
 scyllo-inositol-1-O-yl]acetyl]amino]ethyl]-4-O-(2-methoxy-2-oxoethyl)-,
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 no]hexanoate] (CA INDEX NAME)

Relative stereochemistry.

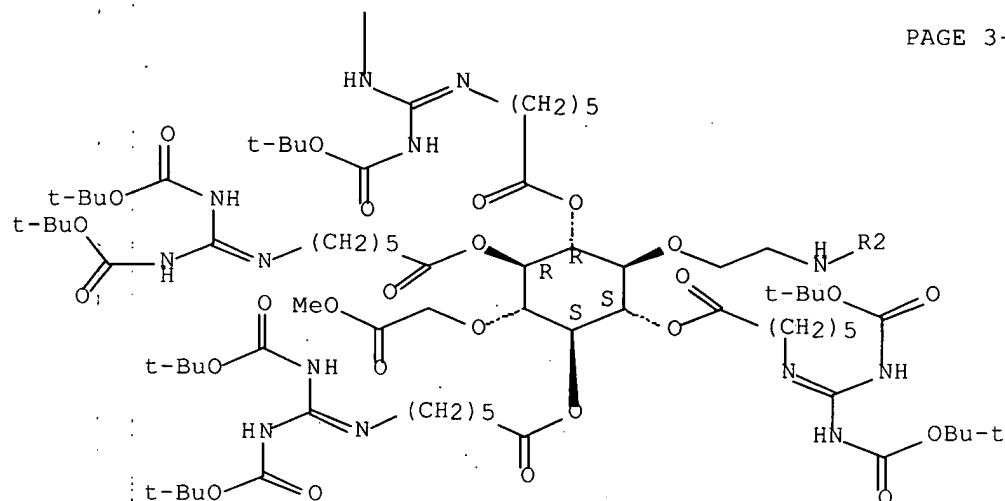
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PAGE 2-A



PAGE 3-A

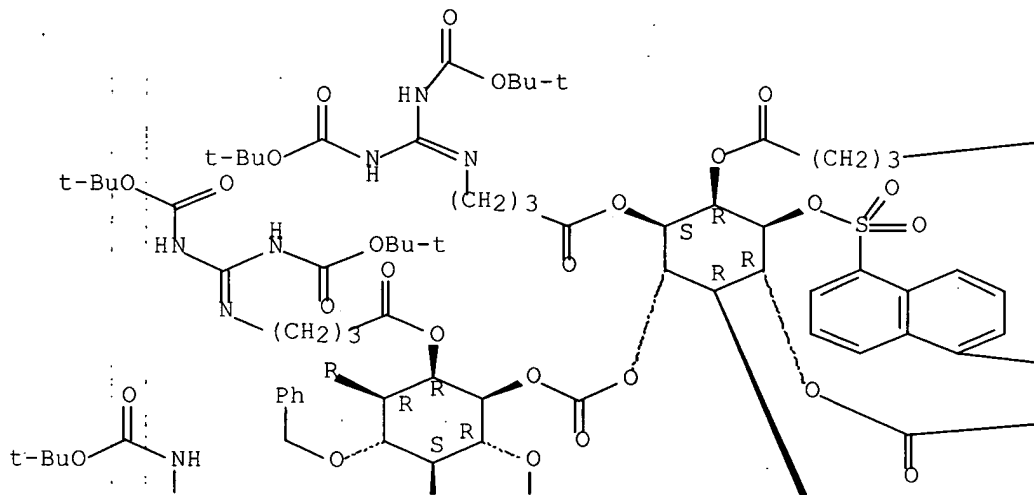


RN 929623-34-7 HCAPLUS

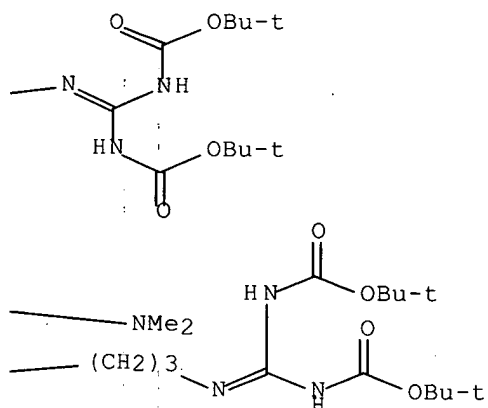
CN myo-Inositol, 4-O-(phenylmethyl)-, 2,3,5,6-tetrakis[4-[[bis[[[(1,1-dimethylethoxy)carbonyl]amino]methylene]amino]butanoate] 1-(hydrogen carbonate), 6-ester with myo-inositol 1,2,4,5-tetrakis[4-[[bis[[[(1,1-dimethylethoxy)carbonyl]amino]methylene]amino]butanoate] 3-[5-(dimethylamino)-1-naphthalenesulfonate] (CA INDEX NAME)

Relative stereochemistry.

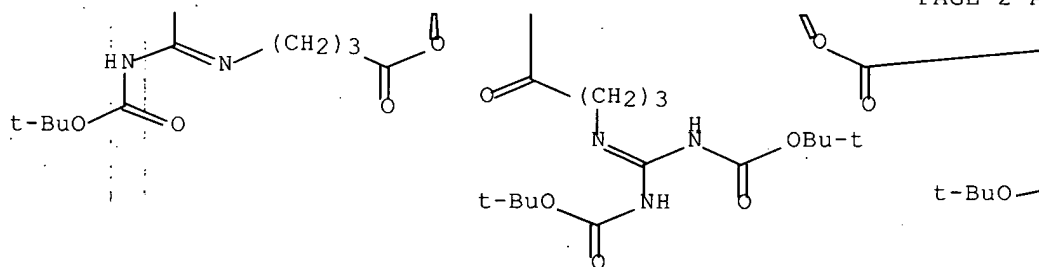
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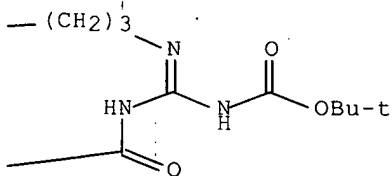
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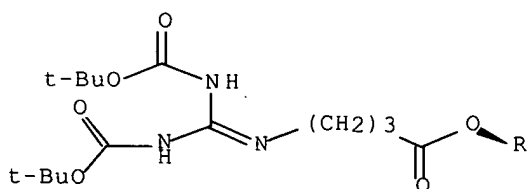
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PAGE 2-B



PAGE 3-A



IT 929623-44-9P 929623-45-0P 929623-46-1P
929708-16-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(design, synthesis, and delivery properties of novel guanidine-containing
mol. transporters built on dimeric inositol scaffolds)

RN 929623-44-9 HCAPLUS

CN scyllo-Inositol, 1-O-[2-[[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-
1(3H),9'-[9H]xanthen]-5-yl)amino]thioxomethyl]amino]ethyl]-4-O-[2-[[2-
[2,3,5,6-tetrakis-O-[4-[(aminoiminomethyl)amino]-1-oxobutyl]-4-O-(2-
methoxy-2-oxoethyl)-scyllo-inositol-1-O-yl]ethyl]amino]-2-oxoethyl]-,
2,3,5,6-tetrakis[4-[(aminoiminomethyl)amino]butanoate],
2,2,2-trifluoroacetate (1:8) (CA INDEX NAME)

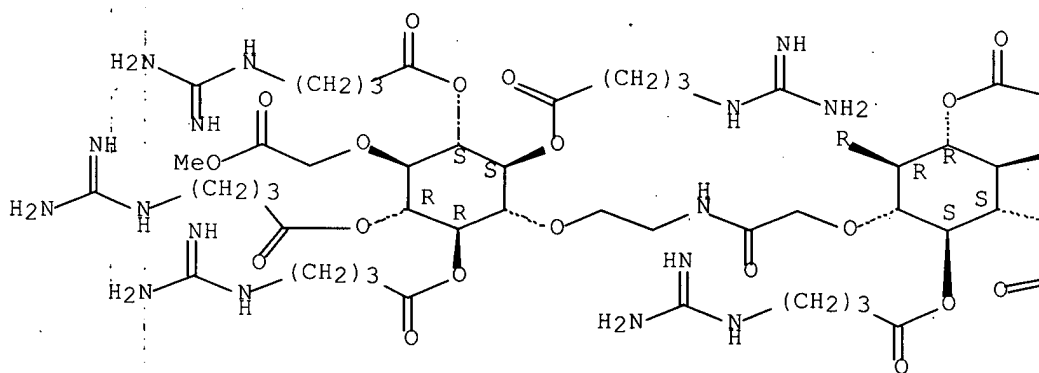
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CRN 898814-85-2

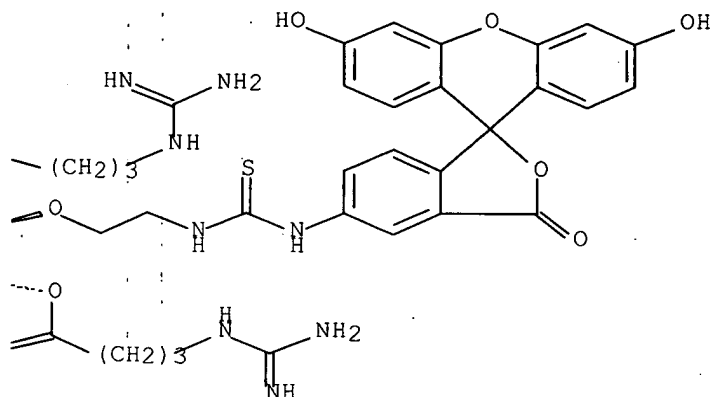
CMF C82 H121 N27 O28 S

Relative stereochemistry.

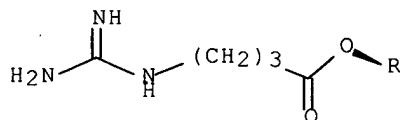
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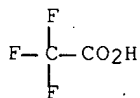
PAGE 2-A



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 929623-45-0 HCAPLUS

CN scyllo-Inositol, 1-O-[2-[[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9']-[9H]xanthen]-5-yl)amino]thioxomethyl]amino]ethyl]-4-O-[2-[[2-[2,3,5,6-tetrakis-O-[6-[(aminoiminomethyl)amino]-1-oxohexyl]-4-O-(2-methoxy-2-oxoethyl)-scyllo-inositol-1-O-yl]ethyl]amino]-2-oxoethyl]-, 2,3,5,6-tetrakis[6-[(aminoiminomethyl)amino]hexanoate], 2,2,2-trifluoroacetate (1:8) (CA INDEX NAME)

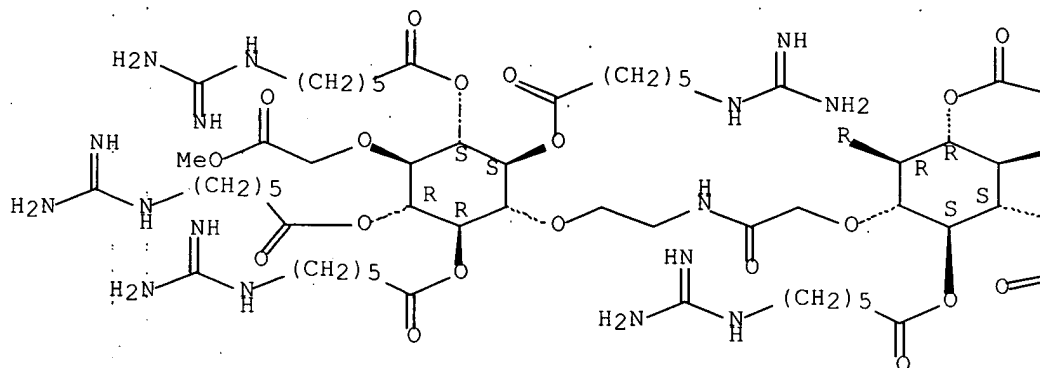
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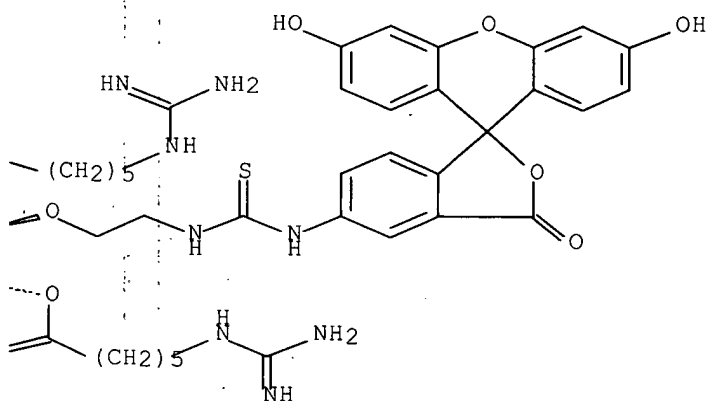
CMF C98 H153 N27 O28 S

Relative stereochemistry.

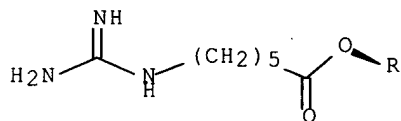
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PAGE 1-B

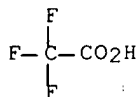


PAGE 2-A



CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 929623-46-1 HCAPLUS

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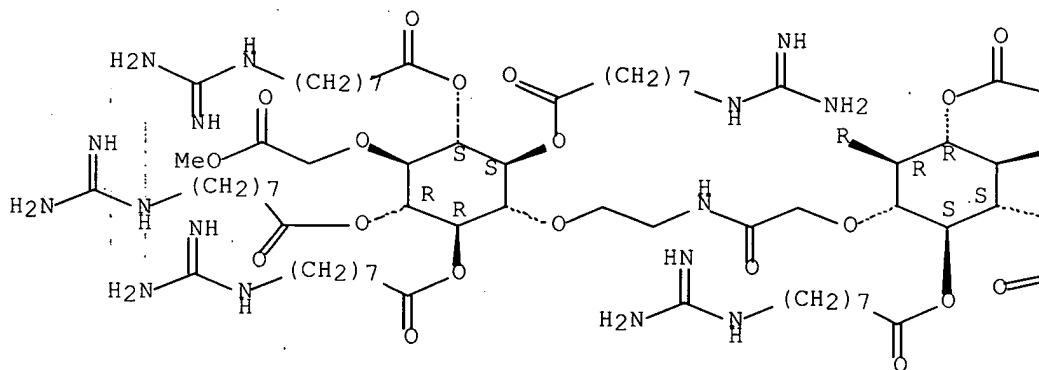
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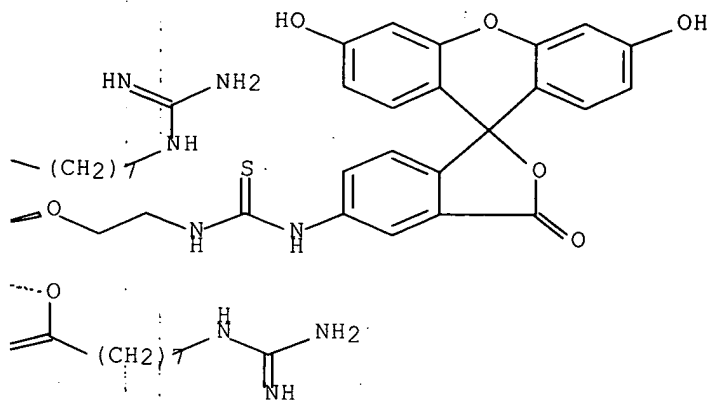
CMF C114 H185 N27 O28 S

Relative stereochemistry.

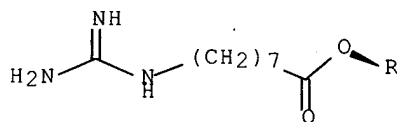
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PAGE 1-B



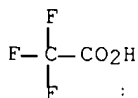
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CM 2

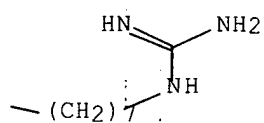
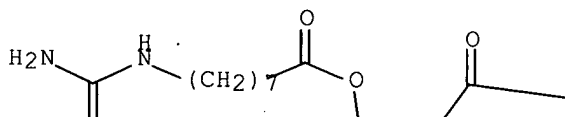
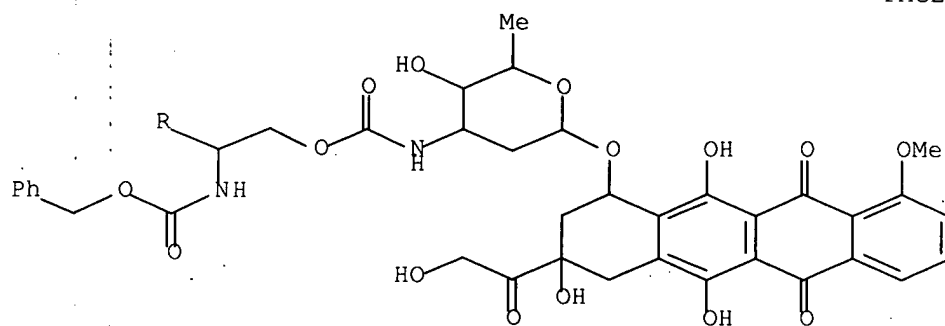
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CMF C2 H F3 O2

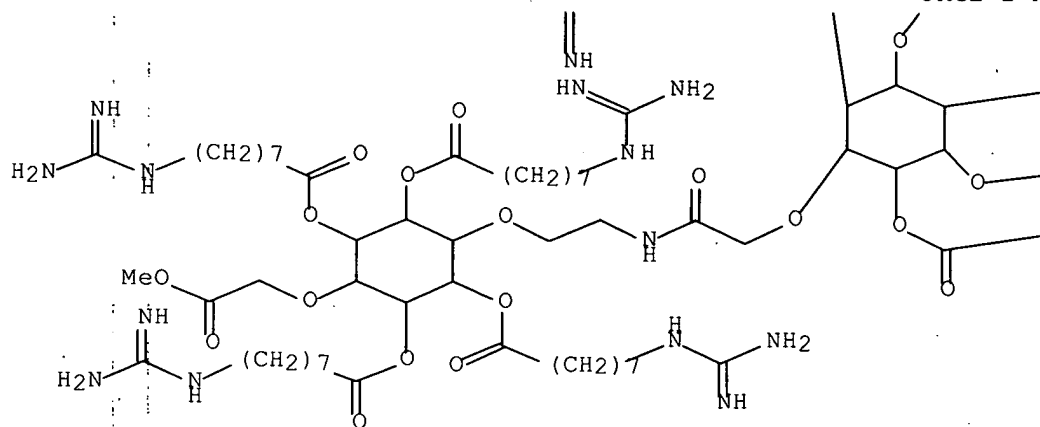


RN 929708-16-7 HCAPLUS

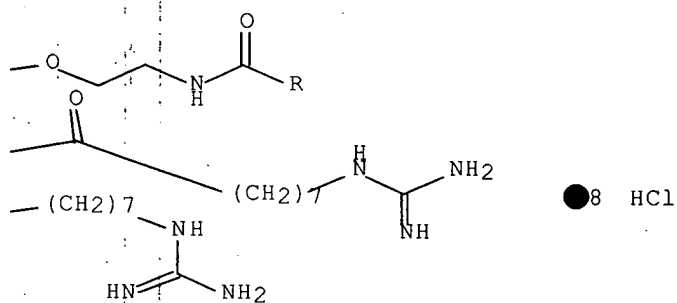
CN scyllo-Inositol, 1-O-[2-[[[(2S)-3-(carboxyoxy)-1-oxo-2-[[[(phenylmethoxy)carbonyl]amino]propyl]amino]ethyl]-4-O-[2-oxo-2-[[2-[2,3,5,6-tetrakis-O-[8-[(aminoiminomethyl)amino]-1-oxooctyl]-4-O-(2-methoxy-2-oxoethyl)-scyllo-inositol-1-O-yl]ethyl]amino]ethyl]-, 2,3,5,6-tetrakis[8-[(aminoiminomethyl)amino]octanoate], amide with (8S,10S)-10-[(3-amino-2,3,6-trideoxy- α -L-lyxo-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy-5,12-naphthacenedione, hydrochloride (1:8) (CA INDEX NAME)



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IT 929623-37-0P 929623-38-1P 929623-40-5P
 929623-41-6P 929623-42-7P 929623-43-8P
 929707-92-6P

RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (fluorescence microscope image; design, synthesis, and delivery
 properties of novel guanidine-containing mol. transporters built on dimeric
 inositol scaffolds)

RN 929623-37-0 HCAPLUS

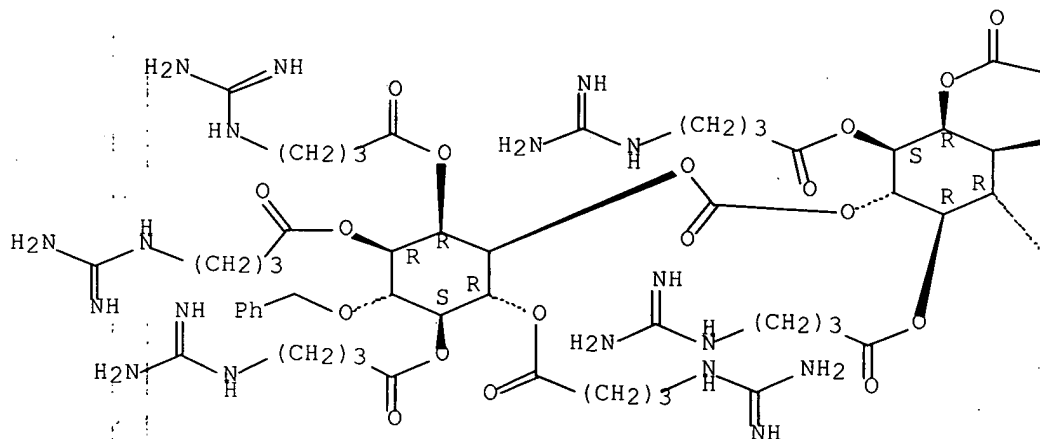
CN myo-Inositol, 4-O-(phenylmethyl)-, 2,3,5,6-tetrakis[4-
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 myo-inositol 1,2,4,5-tetrakis[4-[(aminoiminomethyl)amino]butanoate]
 3-[5-(dimethylamino)-1-naphthalenesulfonate], 2,2,2-trifluoroacetate (1:8)
 (CA INDEX NAME)

CM 1

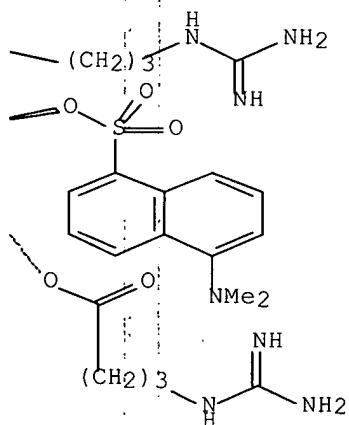
CRN 929623-36-9
 CMF C72 H111 N25 O23 S

Relative stereochemistry.

PAGE 1-A



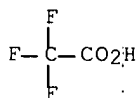
PAGE 1-B



CM 2

CRN: 76-05-1

CMF: C2 H F3 O2



RN 929623-38-1 HCAPLUS

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[(aminoiminomethyl)amino]hexanoate] 1-(hydrogen carbonate), 6-ester with

myo-inositol 1,2,4,5-tetrakis[6-[(aminoiminomethyl)amino]hexanoate]
 3-[5-(dimethylamino)-1-naphthalenesulfonate], 2,2,2-trifluoroacetate (1:8)
 (CA INDEX NAME)

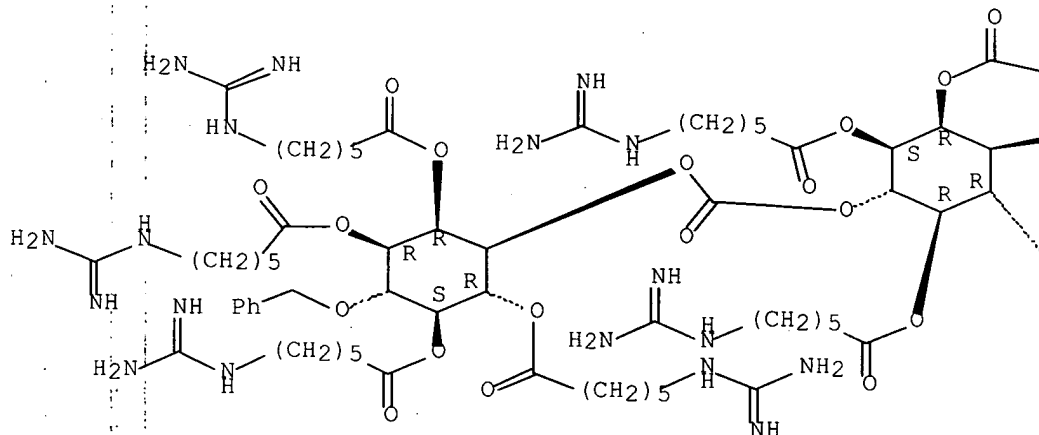
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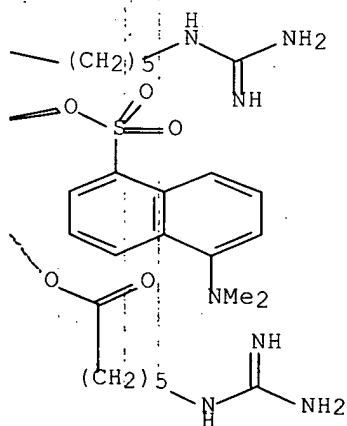
CMF C88 H143 N25 O23 S

Relative stereochemistry.

PAGE 1-A



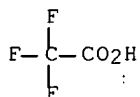
PAGE 1-B



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 929623-40-5 HCAPLUS

CN myo-Inositol, 4-O-(phenylmethyl)-, 2,3,5,6-tetrakis[8-
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 (CA INDEX NAME)

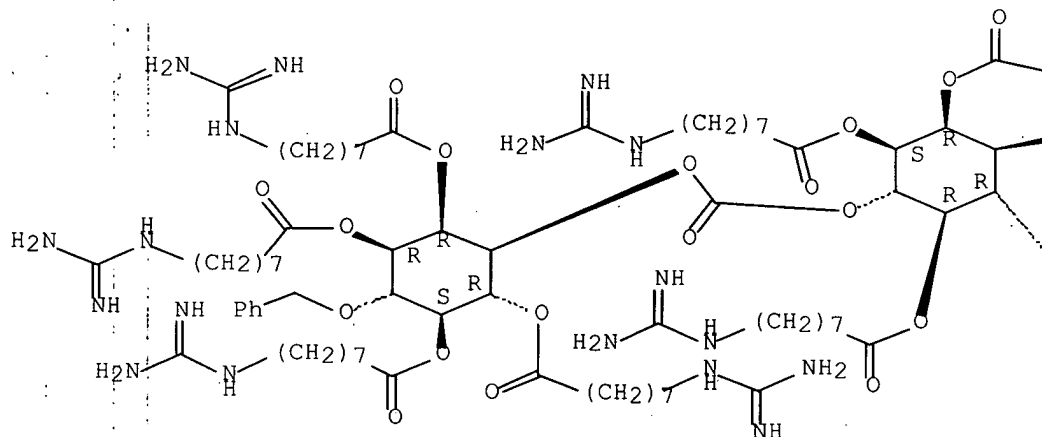
CM 1

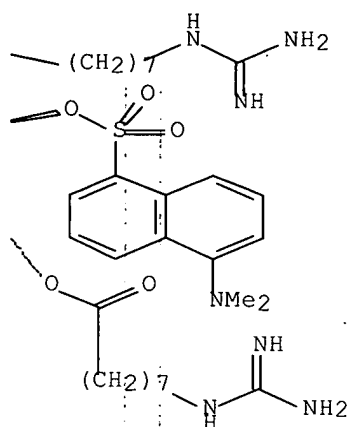
CRN 929623-39-2

CMF C104 H175 N25 O23 S

Relative stereochemistry.

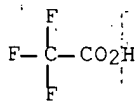
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CM 2

CRN 76-05-1
CMF C2 H F3 O2

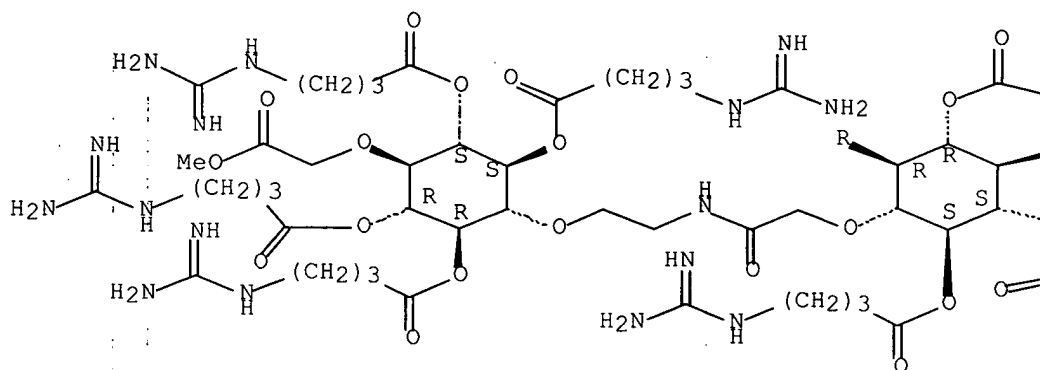


RN 929623-41-6 HCAPLUS

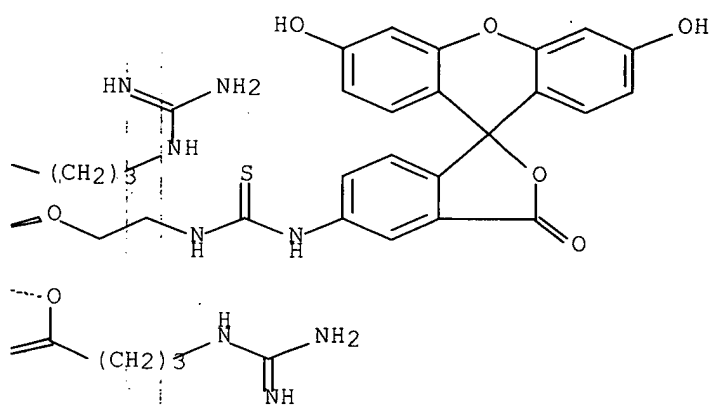
CN scyllo-Inositol, 1-O-[2-[[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)amino]thioxomethyl]amino]ethyl]-4-O-[2-[[2-[2,3,5,6-tetrakis-O-[4-[(aminoiminomethyl)amino]-1-oxobutyl]-4-O-(2-methoxy-2-oxoethyl)-scyllo-inositol-1-O-yl]ethyl]amino]-2-oxoethyl]-, 2,3,5,6-tetrakis[4-[(aminoiminomethyl)amino]butanoate], hydrochloride (1:8) (CA INDEX NAME)

Relative stereochemistry.

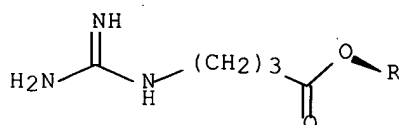
PAGE 1-A



PAGE 1-B



PAGE 2-A



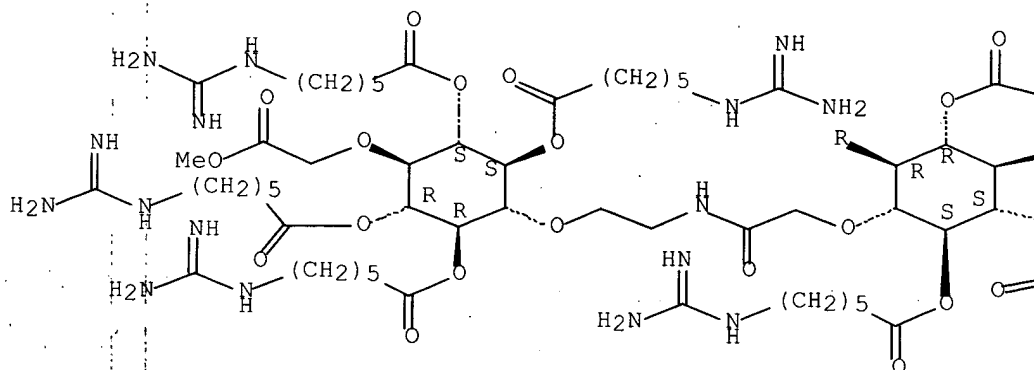
● 8 HCl

RN 929623-42-7 HCAPLUS
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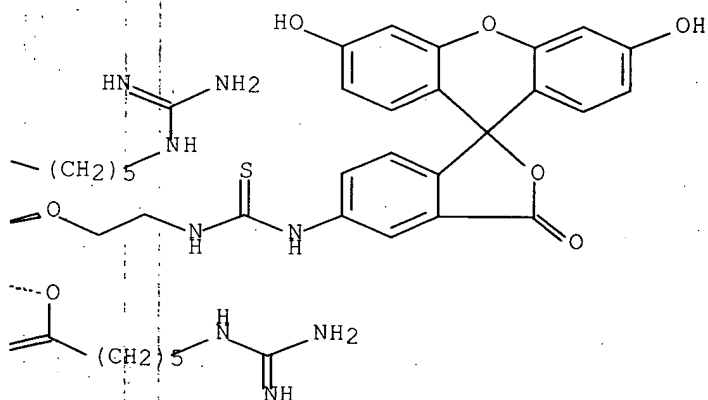
(1:8) (CA INDEX NAME)

Relative stereochemistry.

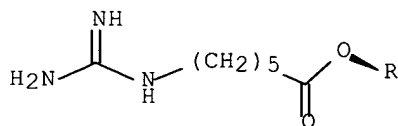
PAGE 1-A



PAGE 1-B



PAGE 2-A



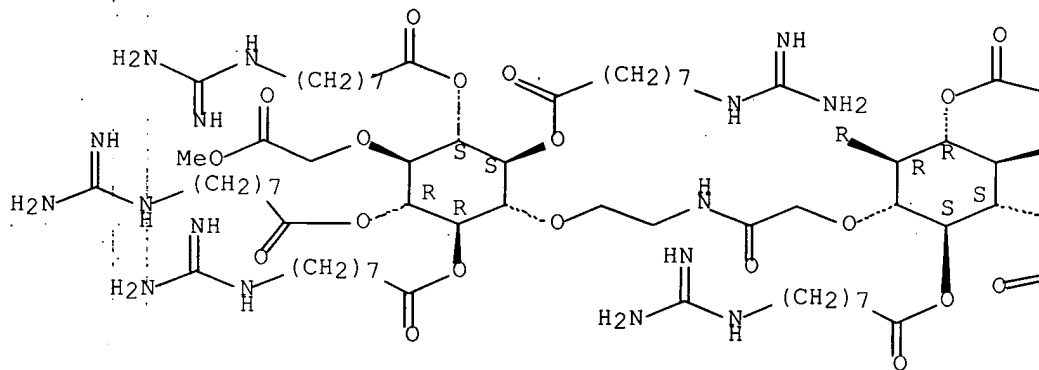
● 8 HCl

RN 929623-43-8 HCAPLUS
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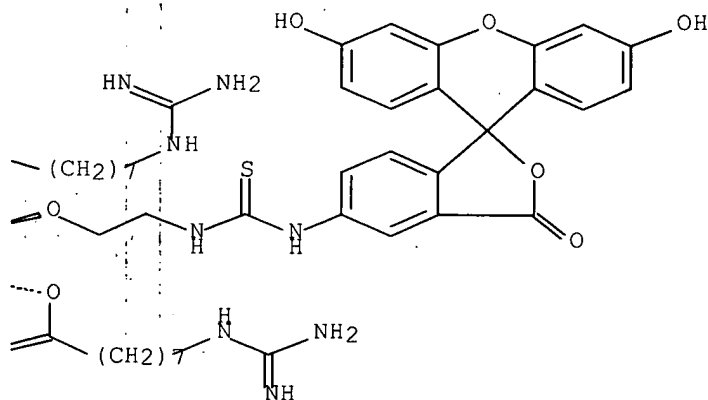
1(3H),9'-[9H]xanthen]-5-yl)amino]thioxomethyl]amino]ethyl]-4-O-[2-[[2-[2,3,5,6-tetrakis-O-[8-[(aminoiminomethyl)amino]-1-oxooctyl]-4-O-(2-methoxy-2-oxoethyl)-scyllo-inositol-1-O-yl]ethyl]amino]-2-oxoethyl]-, 2,3,5,6-tetrakis[8-[(aminoiminomethyl)amino]octanoate], hydrochloride (1:8) (CA INDEX NAME)

Relative stereochemistry.

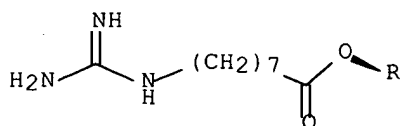
PAGE 1-A



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PAGE 2-A



● 8 HCl

RN 929707-92-6 HCAPLUS
 CN scyllo-Inositol, 2,3,5,6-tetrakis[6-[(aminoiminomethyl)amino]hexanoate] 4-(hydrogen carbonate), 6-ester with scyllo-inositol 1,2,4,5-tetrakis[6-[(aminoiminomethyl)amino]hexanoate] 3-[5-(dimethylamino)-1-naphthalenesulfonate], 2,2,2-trifluoroacetate (1:8) (CA INDEX NAME)

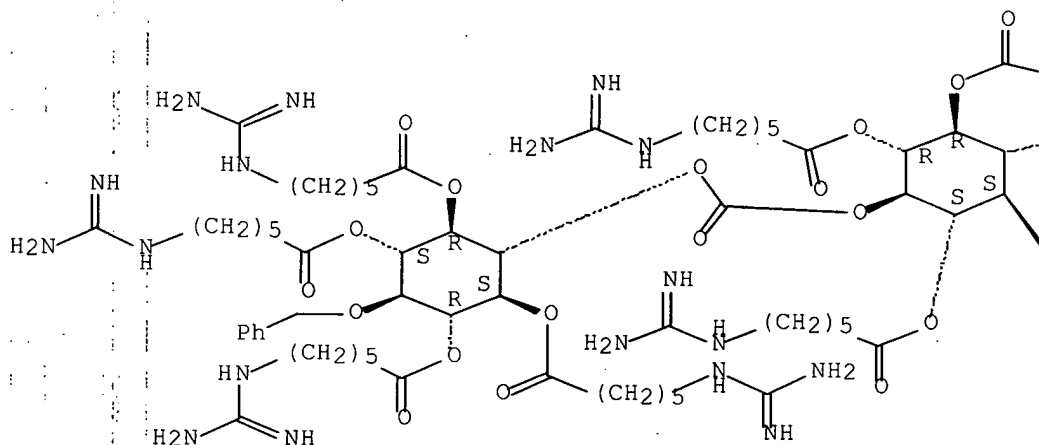
CM 1

CRN 929707-91-5

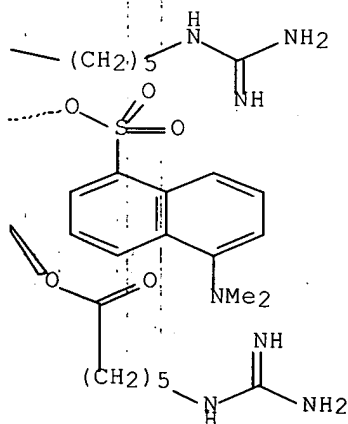
CMF C88 H143 N25 O23 S

Relative stereochemistry.

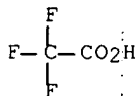
PAGE 1-A



PAGE 1-B



CM 2

CRN: 76-05-1
CMF: C2 H F3 O2

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L137 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:483914 HCAPLUS Full-text

DOCUMENT NUMBER: 145:152384

TITLE: Design, synthesis, and membrane-translocation studies of inositol-based transporters

AUTHOR(S): Maiti, Kaustabh K.; Jeon, Ock-Youm; Lee, Woo Sirl; Kim, Dong-Chan; Kim, Kyong-Tai; Takeuchi, Toshihide; Futaki, Shiroh; Chung, Sung-Kee

CORPORATE SOURCE: Department of Chemistry, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

SOURCE: Angewandte Chemie, International Edition (2006), 45(18), 2907-2912

CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:152384

AB Delivery vehicles: Novel guanidine-containing "transporters" constructed on a dimeric inositol scaffold show significant translocation across the cell membrane and the blood-brain barrier, as well as unique in vitro and in vivo distributions. Doxorubicin was efficiently delivered to mouse-brain tissue by conjugating the compound with such a transporter (see the fluorescence microscopy image).

IT 898814-85-2P 898814-99-8P

RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(design, synthesis, and membrane-translocation studies of inositol-based transporters)

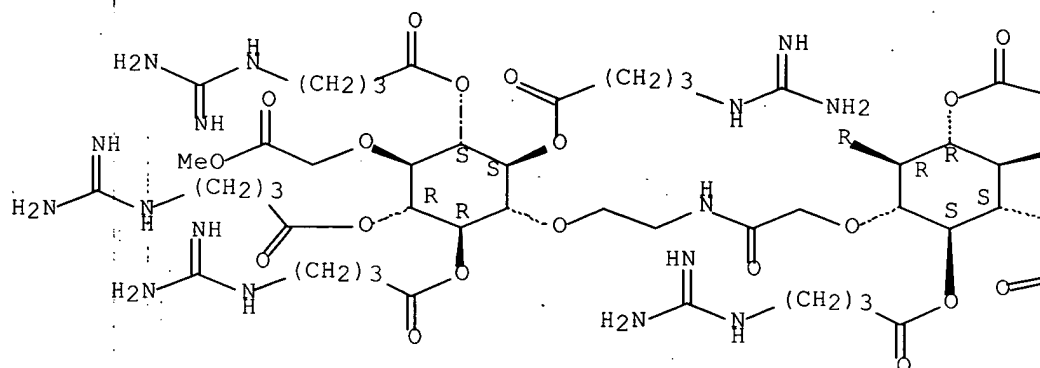
RN 898814-85-2 HCAPLUS

CN scyllo-Inositol, 1-O-[2-[[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9']-[9H]xanthen)-5-yl)amino]carbonyl]amino]ethyl]-4-O-[2-[[2-[2,3,5,6-tetrakis-O-[4-[(aminoiminomethyl)amino]-1-oxobutyl]-4-O-(2-methoxy-2-oxoethyl)-scyllo-inositol-1-O-yl]ethyl]amino]-2-ethyl]-, 2,3,5,6-tetrakis[4-[(aminoiminomethyl)amino]butanoate] (9CI) (CA INDEX NAME)

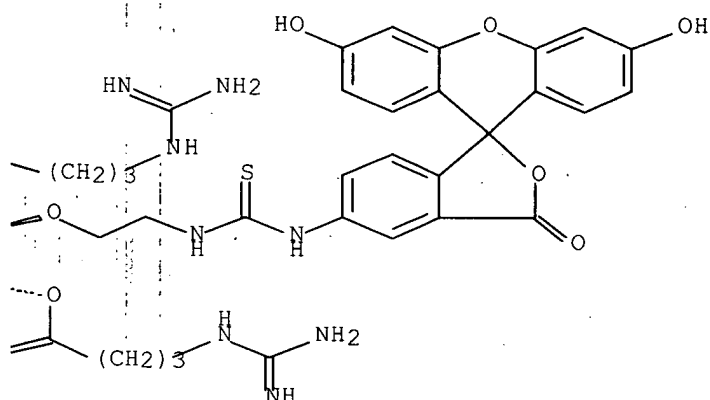
Relative stereochemistry.

POST PRIORITY/FILING

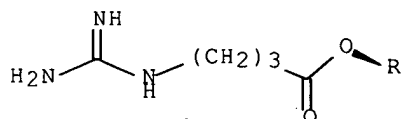
PAGE 1-A



PAGE 1-B



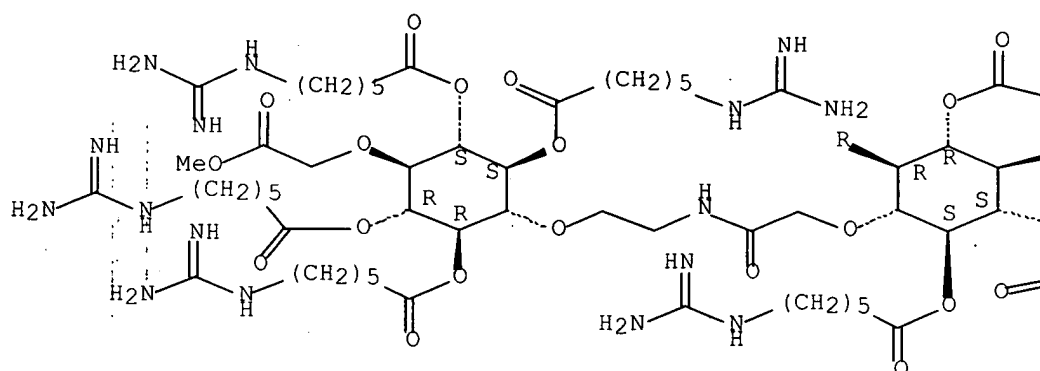
PAGE 2-A



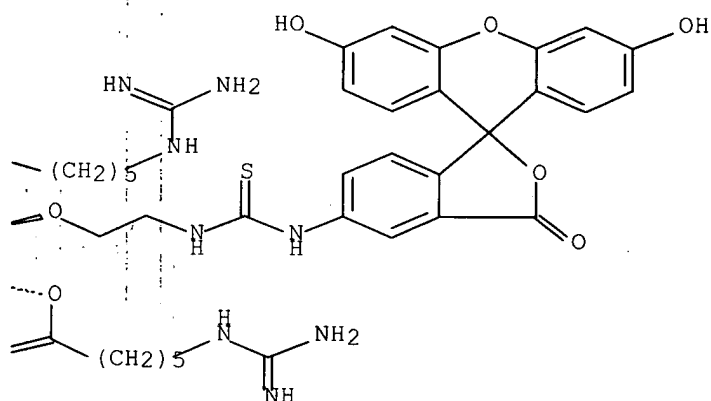
RN 898814-93-2 HCAPLUS
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Relative stereochemistry.

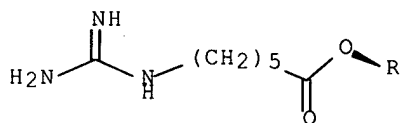
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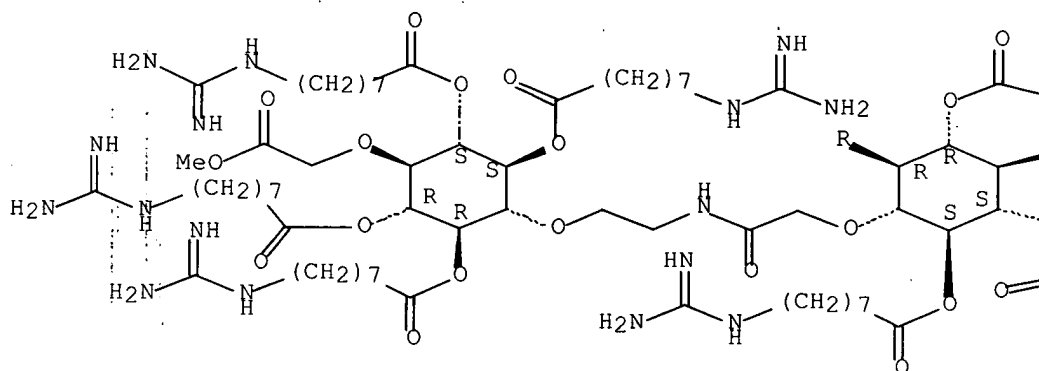
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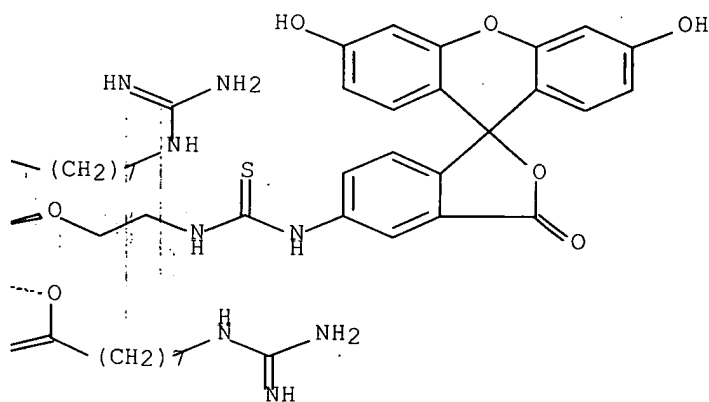
RN 898814-99-8 HCAPLUS
 CN scyllo-Inositol, 1-O-[2-[[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H);9'-[9H]xanthen]-5-yl)amino]carbonyl]amino]ethyl]-4-O-[2-[[2-[2,3,5,6-tetrakis-O-[8-[(aminoiminomethyl)amino]-1-oxooctyl]-4-O-(2-methoxy-2-oxoethyl)-scyllo-inositol-1-O-yl]ethyl]amino]-2-ethyl]-, 2,3,5,6-tetrakis[8-[(aminoiminomethyl)amino]octanoate] (9CI) (CA INDEX NAME)

Relative stereochemistry.

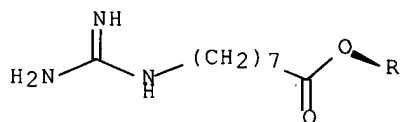
PAGE 1-A



PAGE 1-B



PAGE 2-A



IT 898815-05-9

RL: BSU (Biological study, unclassified); PRP (Properties); THU
(Therapeutic use); BIOL (Biological study); USES (Uses)
(design, synthesis, and membrane-translocation studies of
inositol-based transporters)

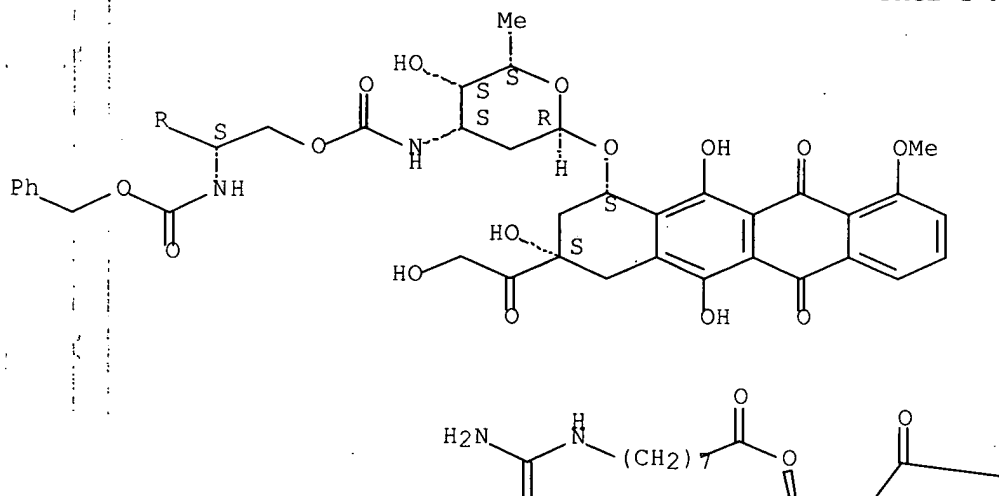
RN 898815-05-9 HCAPLUS

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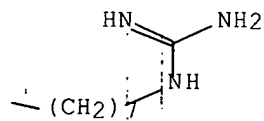
[[(phenylmethoxy) carbonyl] amino] propyl] amino] ethyl]-4-O-[2-oxo-2-[[2-[2,3,5,6-tetrakis-O-[8-[(aminoiminomethyl) amino]-1-oxooctyl]-4-O-(2-methoxy-2-oxoethyl)-D-scyllo-inositol-1-O-yl] ethyl] amino] ethyl]-, 2,3,5,6-tetrakis[8-[(aminoiminomethyl) amino] octanoate], amide with (8S,10S)-10-[(3-amino-2,3,6-trideoxy- α -L-lyxo-hexopyranosyl) oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy-5,12-naphthacenedione (CA INDEX NAME)

Absolute stereochemistry.

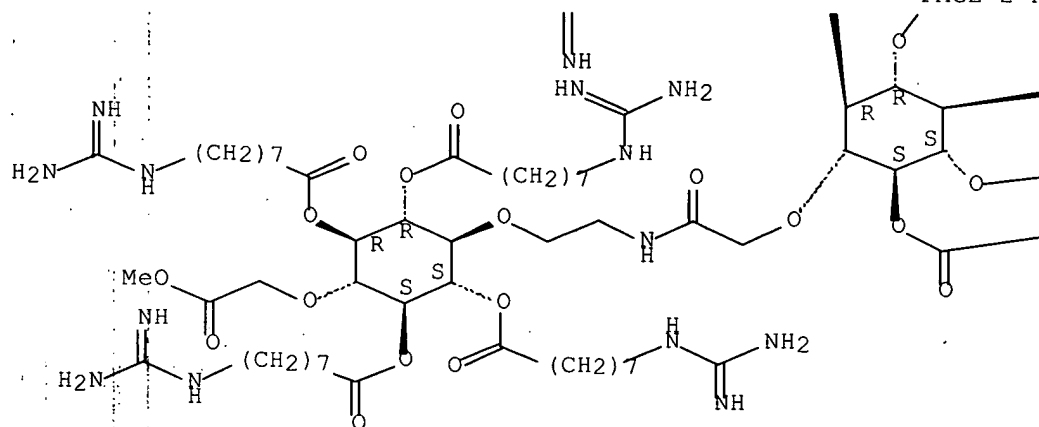
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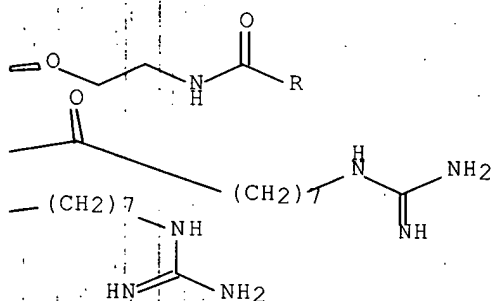
PAGE 1-B



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IT 898815-49-1P 898815-54-8P 898815-81-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

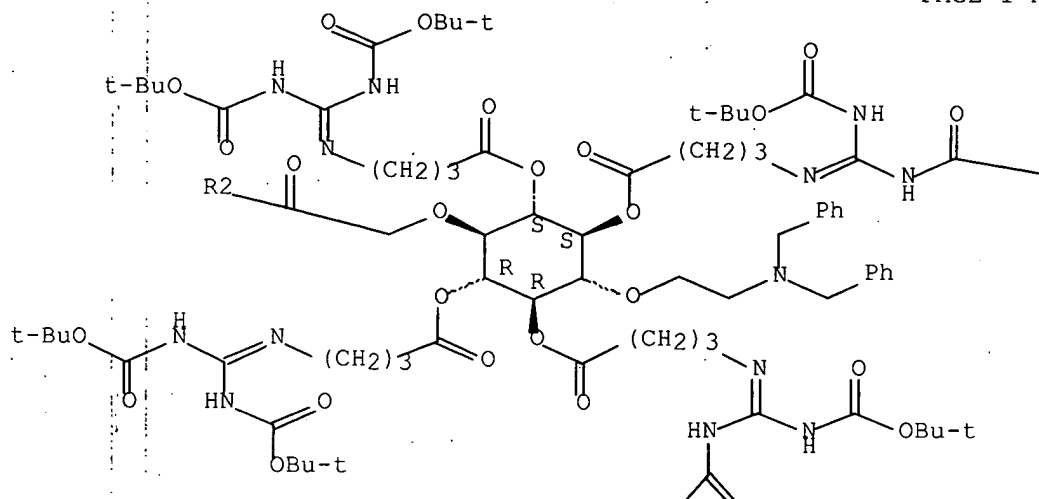
(design, synthesis, and membrane-translocation studies of inositol-based transporters)

RN 898815-49-1 HCAPLUS

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Relative stereochemistry.

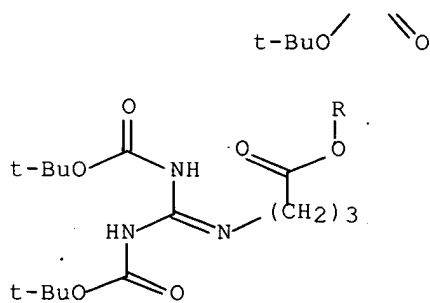
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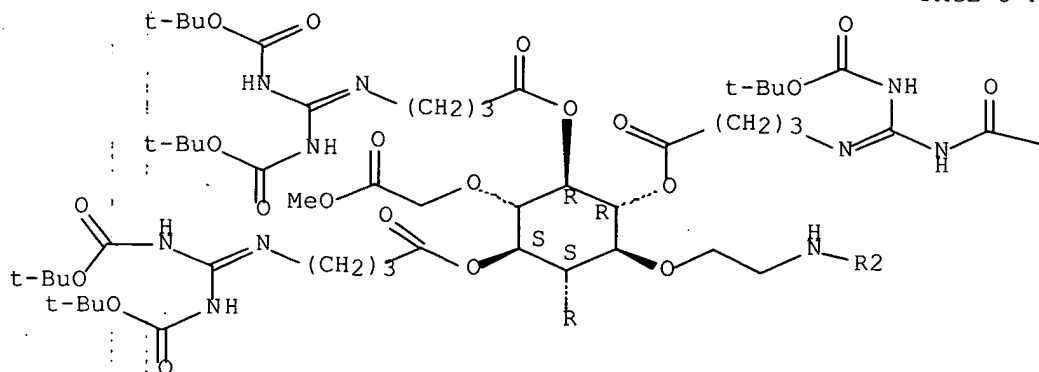
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-OBu-t

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PAGE 3-A



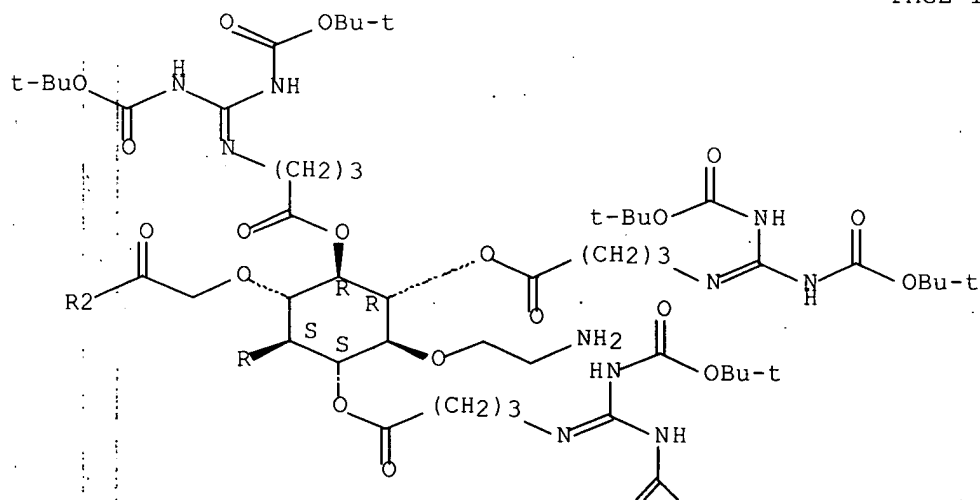
PAGE 3-B

—OBu-t

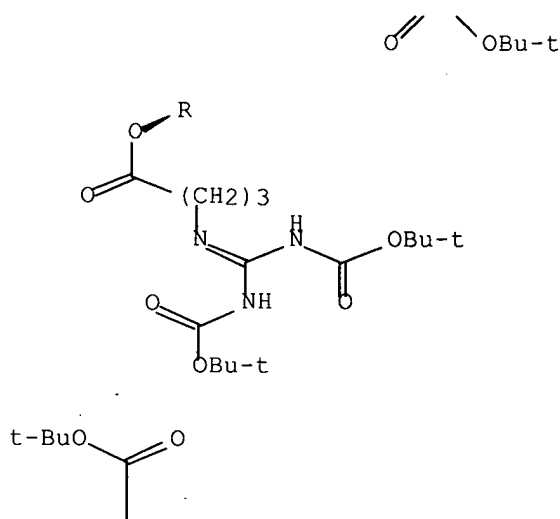
RN 898815-54-8 HCAPLUS
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scyllo-inositol-1-O-yl]acetyl]amino]ethyl]-4-O-(2-methoxy-2-oxoethyl)-,
2,3,5,6-tetrakis[4-[[bis[[[(1,1-dimethylethoxy)carbonyl]amino]methylene]ami
no]butanoate] (CA INDEX NAME)

Relative stereochemistry.

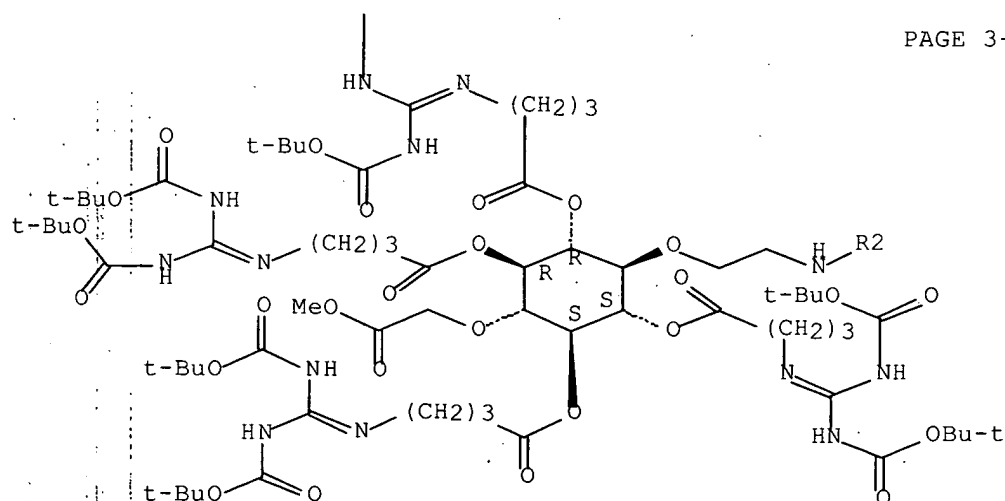
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PAGE 2-A

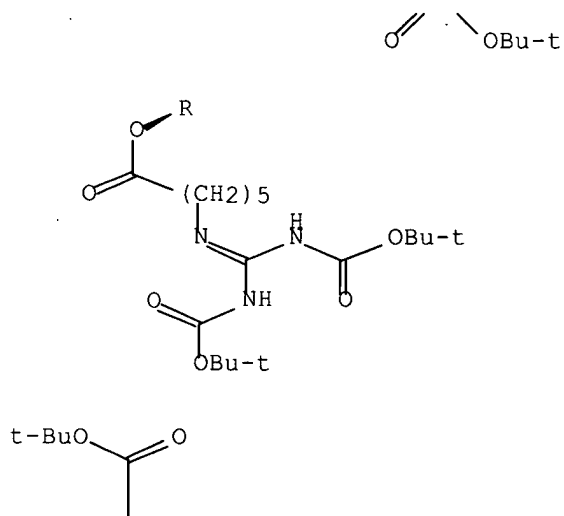
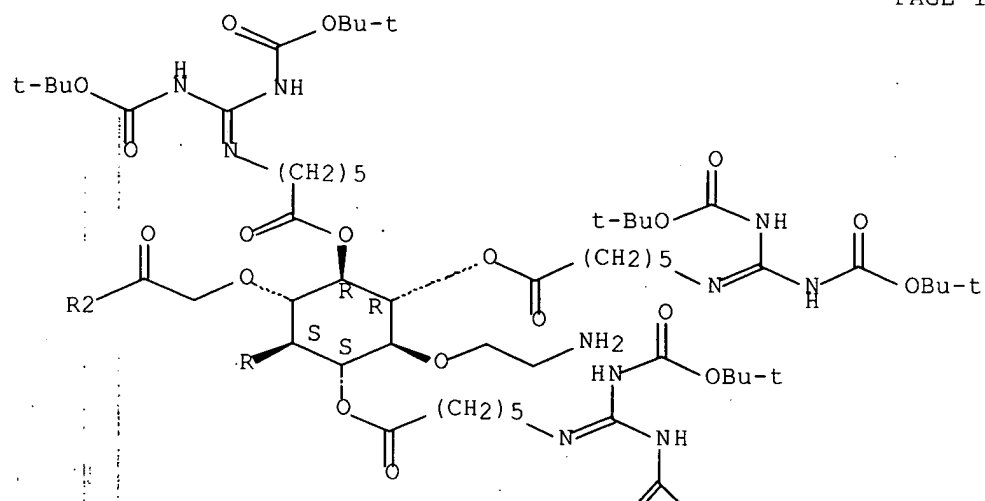


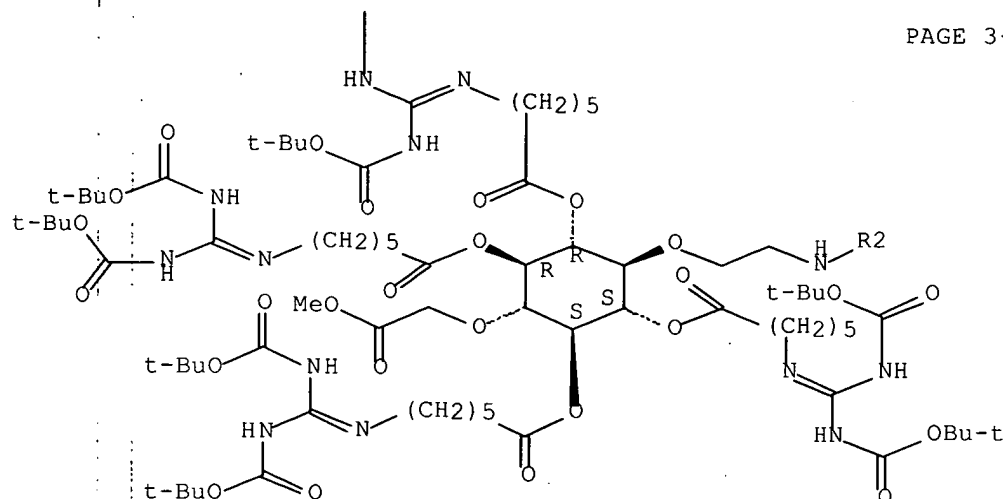
PAGE 3-A



RN 898815-81-1 HCAPLUS
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 [[bis[[(1,1-dimethylethoxy)carbonyl]amino]methylene]amino]-1-oxohexyl]-
 scyllo-inositol-1-O-yl]acetyl]amino]ethyl]-4-O-(2-methoxy-2-oxoethyl)-,
 2,3,5,6-tetrakis[6-[[bis[[(1,1-dimethylethoxy)carbonyl]amino]methylene]ami
 no]hexanoate] (CA INDEX NAME)

Relative stereochemistry.





REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L137. ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:1004682 HCAPLUS Full-text
 DOCUMENT NUMBER: 143:306498

TITLE: Inositol-based molecular transporters and processes for the preparation thereof

INVENTOR(S): Chung, Sung-Kee; Jeon, Ock-Younm; Maiti, Kaustabh Kumar; Yu, Seok-Ho

PATENT ASSIGNEE(S): Postech Foundation, S. Korea

SOURCE: PCT Int. Appl., 58 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085159	A1	20050915	WO 2004-KR1982	20040806
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
KR 2005089422	A	20050908	KR 2004-14833	20040305
EP 1678110	A1	20060712	EP 2004-748517	20040806
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JP 2007523889	T	20070823	JP 2006-546800	20040806
US 2006280796	A1	20061214	US 2006-565164	20060119

This is WIPO of my Applic.

PRIORITY APPLN. INFO.:

KR 2004-14833

A 20040305

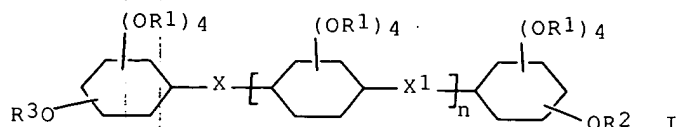
WO 2004-KR1982

W 20040806

OTHER SOURCE(S):

MARPAT 143:306498

GI



AB Inositol derivs. I, wherein R1 is CO(CH₂)_p-NH-C(:NH)-NH₂, p is 1-12; R2 and R3 are independently H, alkyl, arylalkyl, cycloalkyl, heteroalkyl, alkylamine, acyl, alkyl-carboxylate, sulfonyl; n is 0-2; X and X1 are independently O-CO-O, O-CO-NH-(CH₂)_m-O; O-CO, (CH₂)_q-O, O-(CH₂)_q-CO-NH-(CH₂)_m-O; q is 1-5, were prepared and are effective in significantly enhancing the transportation of various therapeutic mols. across a biol. membrane, which may include the plasma membrane, nuclear membrane or blood-brain barrier. Thus, 4-O-(2-aminoethyl)-1-O- (methyloxycarbonylmethyl)-2,3:5,6-di-O-isopropylidene-scylo-inositol was prepared and tested as mol. transporter of various therapeutic mols. across a biol. membrane.

IT 863892-13-1P 863892-14-2P

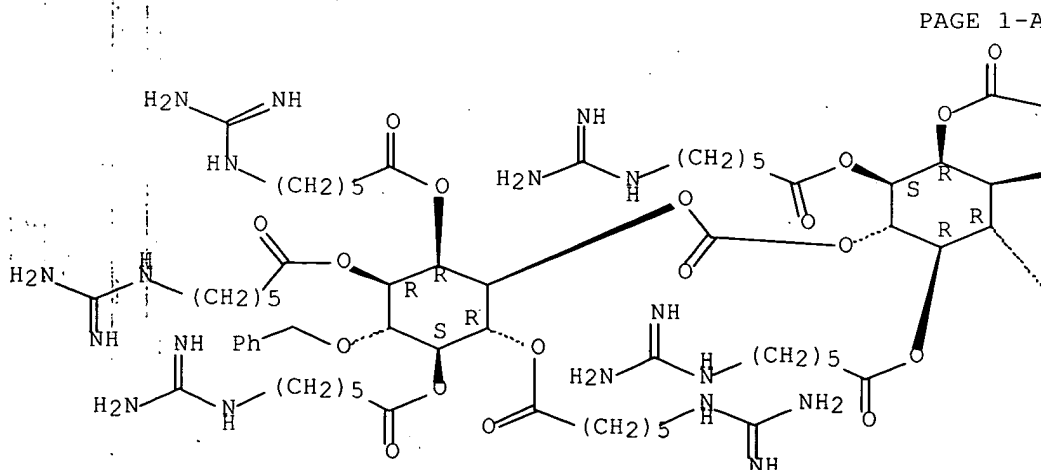
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(inositol-based mol. transporters and processes for the preparation thereof)

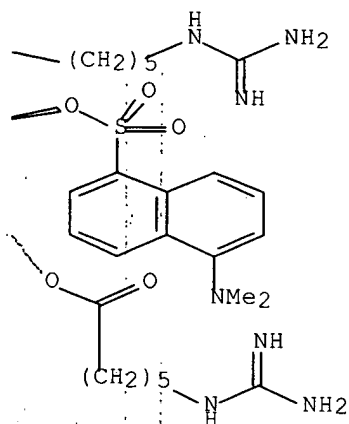
RN 863892-13-1 HCAPLUS

CN myo-Inositol, 4-O-(phenylmethyl)-, 2,3,5,6-tetrakis[6-[(aminoiminomethyl)amino]hexanoate] 1-(hydrogen carbonate), ester with myo-inositol 1,2,4,5-tetrakis[6-[(aminoiminomethyl)amino]hexanoate] 3-[5-(dimethylamino)-1-naphthalenesulfonate] (9CI) (CA INDEX NAME)

Relative stereochemistry.



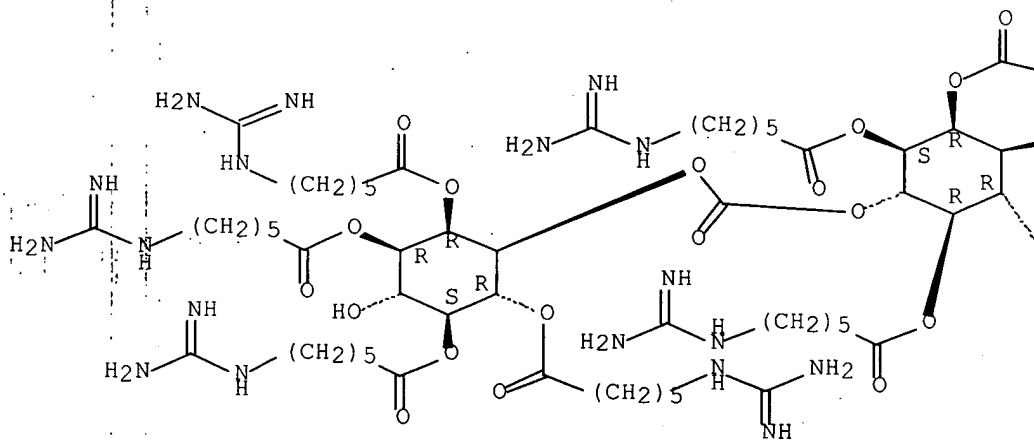
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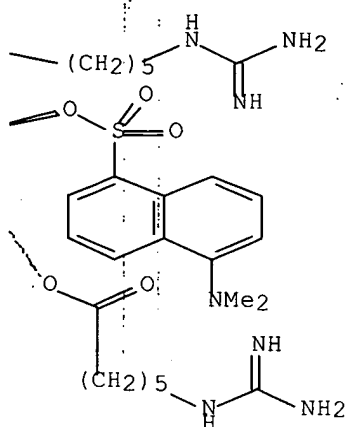


RN 863892-14-2 HCAPLUS

CN myo-Inositol, 1,2,4,5-tetrakis[6-[(aminoiminomethyl)amino]hexanoate]
6-(hydrogen carbonate) 3-[5-(dimethylamino)-1-naphthalenesulfonate],
3-ester with myo-inositol 1,2,4,5-tetrakis[6-[(aminoiminomethyl)amino]hexa
noate] (9CI) (CA INDEX NAME)

Relative stereochemistry.





IT 863892-12-0P

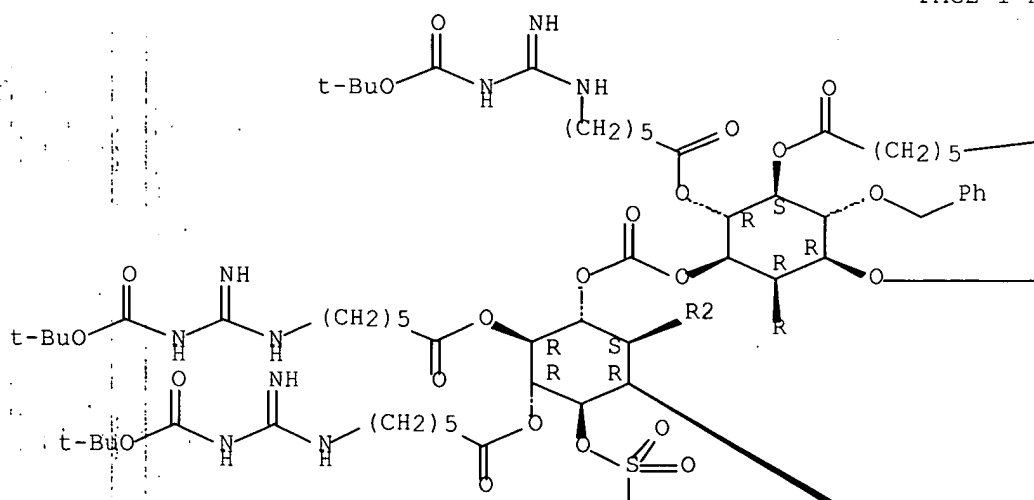
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(inositol-based mol. transporters and processes for the preparation thereof)

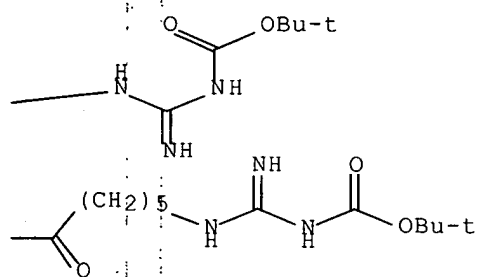
RN 863892-12-0 HCAPLUS

CN myo-Inositol, 4-O-(phenylmethyl)-, 2,3,5,6-tetrakis[6-[[[(1,1-dimethylethoxy)carbonyl]amino]iminomethyl]amino]hexanoate] 1-(hydrogen carbonate), ester with myo-inositol 1,2,4,5-tetrakis[6-[[[(1,1-dimethylethoxy)carbonyl]amino]iminomethyl]amino]hexanoate] 3-[5-(dimethylamino)-1-naphthalenesulfonate] (9CI) (CA INDEX NAME)

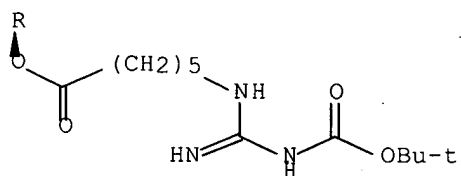
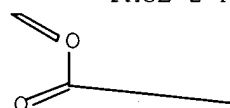
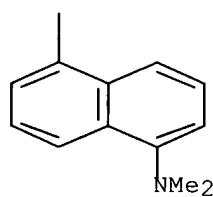
Relative stereochemistry.



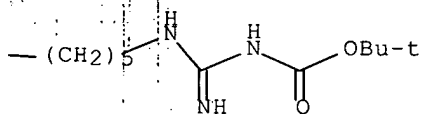
PAGE 1-B



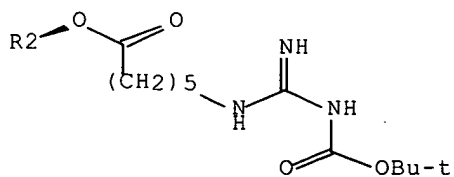
PAGE 2-A



PAGE 2-B



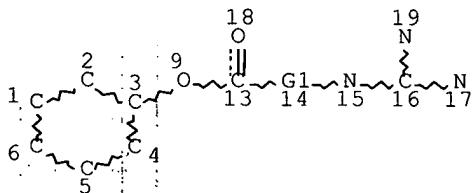
PAGE 3-A



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD: ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> => d stat que l148

L132 STR



REP G1=(1-12) C

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

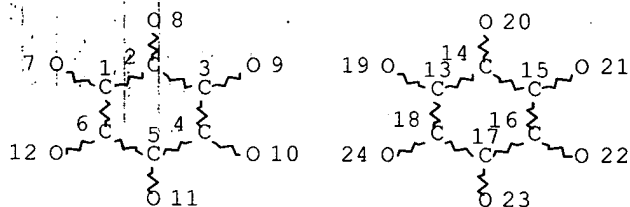
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L134 383 SEA FILE=REGISTRY SSS FUL L132

L135 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

L136 26 SEA FILE=REGISTRY SUB=L134 SSS FUL L135

L137 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L136

L138 292 SEA FILE=HCAPLUS ABB=ON PLU=ON "CHUNG SUNG"/AU OR "CHUNG
SUNG KEE"/AU OR CHUNG S/AU OR CHUNG S K?/AU

L139 5 SEA FILE=HCAPLUS ABB=ON PLU=ON "JEON O Y"/AU OR ("JEON OCK
YOUNM"/AU OR "JEON OCK YOUNM"/AU)

L140 1574 SEA FILE=HCAPLUS ABB=ON PLU=ON KUMAR K/AU OR KUMAR K ?/AU

L141 540 SEA FILE=HCAPLUS ABB=ON PLU=ON "YU SEOK"/AU OR "YU SEOK
HO"/AU OR YU S/AU OR YU S H?/AU

L142 16 SEA FILE=HCAPLUS ABB=ON PLU=ON L138 AND (L139 OR L140 OR

L141)
 L143 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L139 AND (L140 OR L141)
 L144 0 SEA FILE=HCAPLUS ABB=ON PLU=ON L140 AND L141
 L145 357 SEA FILE=REGISTRY ABB=ON PLU=ON L134 NOT L136
 L146 720 SEA FILE=HCAPLUS ABB=ON PLU=ON L145
 L147 1 SEA FILE=HCAPLUS ABB=ON PLU=ON (L138 OR L139 OR L140 OR
 L141) AND L146
 L148 13 SEA FILE=HCAPLUS ABB=ON PLU=ON (L142 OR L143 OR L144 OR
 L147) NOT L137

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=> d ibib abs hitstr l148 1-13

L148 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2007:986589 HCAPLUS Full-text

TITLE: Divergent Synthesis of All Possible Optically Active
 Regioisomers of Myo-Inositol Mono- and Bisphosphates
 AUTHOR(S): Seo, Kyung-Chang; Yu, Seok-Ho; Chung,
 Sung-Kee

CORPORATE SOURCE: Department of Chemistry, Pohang University of Science
 & Technology, Pohang, S. Korea

SOURCE: Journal of Carbohydrate Chemistry (2007), 26(5&6),
 305-327

CODEN: JCACDM; ISSN: 0732-8303

PUBLISHER: Taylor & Francis, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB All possible optically active regioisomers of myo-inositol mono- and bis-
 phosphates were synthesized using inositol derivs. suitably protected with
 various protecting groups (IRns) as key intermediates. A series of procedures
 including Novozym 435 catalyzed enzymic resolution of (3aR,4S,7S,7aR)-rel-
 3a,4,7,7a-tetrahydro-2,2-dimethyl-1,3-benzodioxole-4,7- diol diacetate,
 several protection and deprotection reactions, and acyl migration afforded two
 enantiomeric pairs of IR5 and six enantiomeric pairs of IR4. Phosphorylation
 of these key intermediates by the phosphitylation and oxidation procedure gave
 the target products after removal of the protecting groups.

IT INDEXING IN PROGRESS

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L148 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2007:319217 HCAPLUS Full-text

TITLE: Construction of sphingolipids libraries and their
 utilities

AUTHOR(S): Park, Jeong-Ju; Yu, Seok-Ho; Chung,
 Sung-Kee

CORPORATE SOURCE: Department of Chemistry, Pohang University of Science
 and Technology, Pohang, 790-784, S. Korea

SOURCE: International Journal of the Society of Materials
 Engineering for Resources (2006), 14(1/2), 18-21
 CODEN: IMEREB; ISSN: 1347-9725

PUBLISHER: Society of Materials Engineering for Resources of
 Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

POST FILING/PRIORITY

POST FILING/PRIORITY

AB Sphingolipids such as ceramide and glycosylceramide have recently attracted intense research interests because of their roles as signalling molcs. in many important physiol. processes, such as apoptosis, inflammation and immune responses. Their well-defined modular structures are ideally amenable to library formation for medicinal chemical investigations. We have developed practical, divergent synthetic routes to sphingosine and phytosphingosine isomers as well as to carba-sugar analogs of all D-aldohepyranose isomers toward these goals. And then we have proceeded to prepare ceramide libraries, composed of more than 500 compds. each, based on these sphingosine and phytosphingosine isomers, and demonstrated their utility in cell-based bioassays involving activation of NF- κ B and induction of apoptosis. We are also in the process of forming libraries of mono-glycosylceramide and mono-carba- glycosylceramide.

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L148 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2007:105547 HCAPLUS Full-text POST FILING/PRIORITY

TITLE: Design, synthesis, and delivery properties of novel guanidine-containing molecular transporters built on dimeric inositol scaffolds

AUTHOR(S): Maiti, K. K.; Jeon, O.-Y.; Lee, W. S.; Chung, S.-K.

SOURCE: Chemistry--A European Journal (2007), 13(3), No pp. given

CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal; Errata

LANGUAGE: English

AB Unavailable

L148 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1322934 HCAPLUS Full-text POST FILING/PRIORITY

DOCUMENT NUMBER: 146:229525

TITLE: Practical syntheses of optically active carbagalactose and their potential application to the carbocyclic analogues of KRN7000

AUTHOR(S): Yu, Seok-Ho; Park, Jeong-Ju; Chung, Sung-Kee

CORPORATE SOURCE: Department of Chemistry, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

SOURCE: Tetrahedron: Asymmetry (2006), 17(21), 3030-3036

CODEN: TASYE3; ISSN: 0957-4166

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 146:229525

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Carba- α - and β -D-galactose derivs. were efficiently prepared from a cyclohex-3-ene-1,2-diol derivative I. Regioselective inversion of 2-OH, and stereoselective dihydroxylation of I were accomplished to provide a carba- β -D-

galactose derivative II in a good yield and with a high stereoselectivity. Stereo-inversion of 1-OH of II via oxidation/reduction gave carba- α -D-galactose derivative III with a high stereoselectivity. An efficient coupling of carba- α -galactose III with an aziridine derivative of sphingosine has been demonstrated to give 1-O-carba- α -galactosyl sphingosine derivative IV.

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L148 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1155705 HCAPLUS Full-text

DOCUMENT NUMBER: 145:471812

TITLE: Preparation of glycoside, oligosaccharide and cyclitol molecular transporter analogs with high permeability through biological membranes

INVENTOR(S): Chung, Sung-Kee; Maiti, Kaustabh Kumar; Lee, Woo Sirl; Jeon, Ock-Youm; Yu, Seok-Ho

PATENT ASSIGNEE(S): Postech Foundation, S. Korea; Postech Academy-Industry Foundation

SOURCE: PCT Int. Appl., 74pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006115312	A1	20061102	WO 2005-KR2040	20050629
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
KR 2006112791	A	20061102	KR 2005-35410	20050428

PRIORITY APPLN. INFO.:

KR 2005-35410 A 20050428

OTHER SOURCE(S): MARPAT 145:471812

GI

OR1
OR3
OR3
OR3
OR3
OR2 I

OR1
OR1
R10
OR1
OR1
OR1 II

AB Title compds. I, wherein R1 and R2 are independently H, alkyl, arylalkyl, cycloalkyl, etc.; R3 is a ketoalkylamino guanidine analog are prepared as mol. transporter analogs with permeability for biol. active mols. Thus, II (R1 is -CO-(CH₂)₅NH-C(=NH)-NH₂ hydrochloride salt) was prepared and tested for membrane permeability via fluorescent imaging (no data). In general, I displays good permeability when measured against an arginine nonamer for crossing biol. membrane such as a plasma membrane, nuclear membrane and blood-brain barrier.

IT 913834-26-1P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);

BIOL (Biological study); PREP (Preparation)

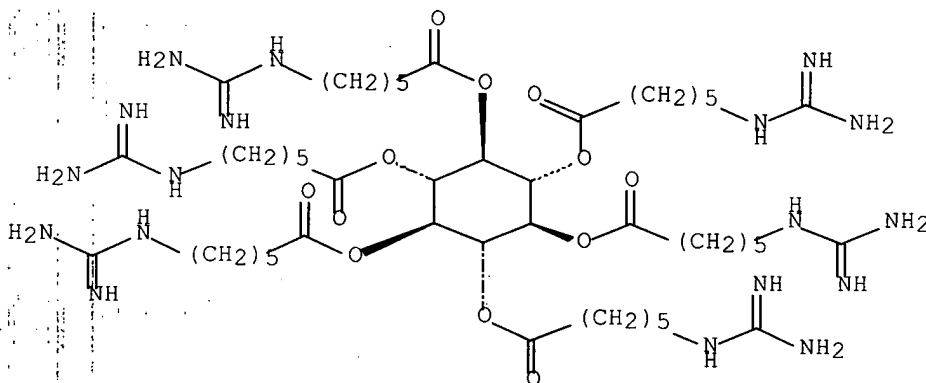
(preparation of glycoside, oligosaccharide and cyclitol mol. transporter analogs with high permeability through biol. membranes)

RN 913834-26-1 HCAPLUS

CN scyllo-Inositol, hexakis[6-[(aminoiminomethyl)amino]hexanoate], hexahydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

● 6 HCl

IT 913834-24-9P 913834-25-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

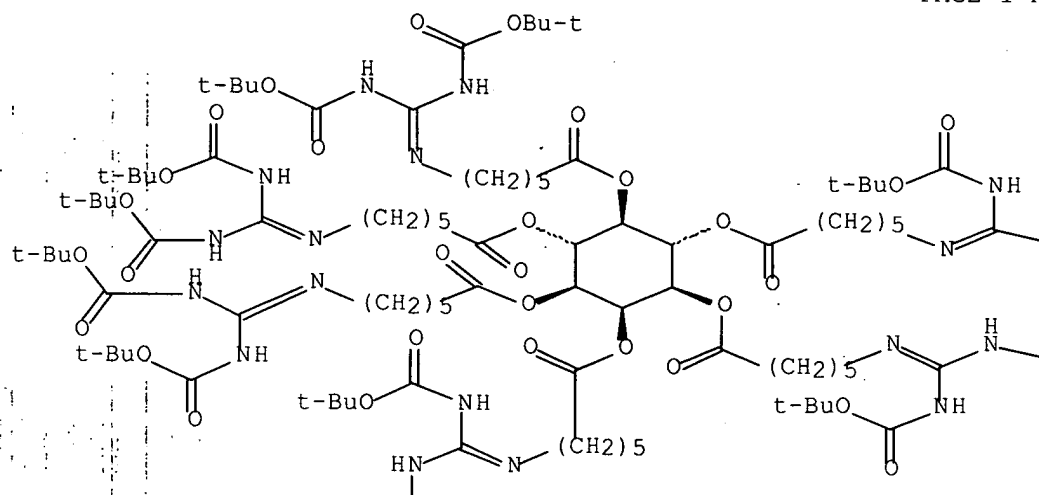
(preparation of glycoside, oligosaccharide and cyclitol mol. transporter analogs with high permeability through biol. membranes)

RN 913834-24-9 HCAPLUS

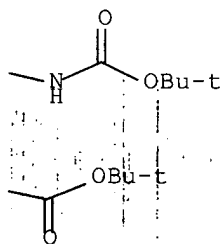
CN myo-Inositol, hexakis[6-[[bis[[[(1,1-dimethylethoxy)carbonyl]amino]methylene]amino]hexanoate] (9CI) (CA INDEX NAME)

Relative stereochemistry.

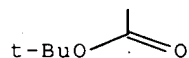
PAGE 1-A



PAGE 1-B



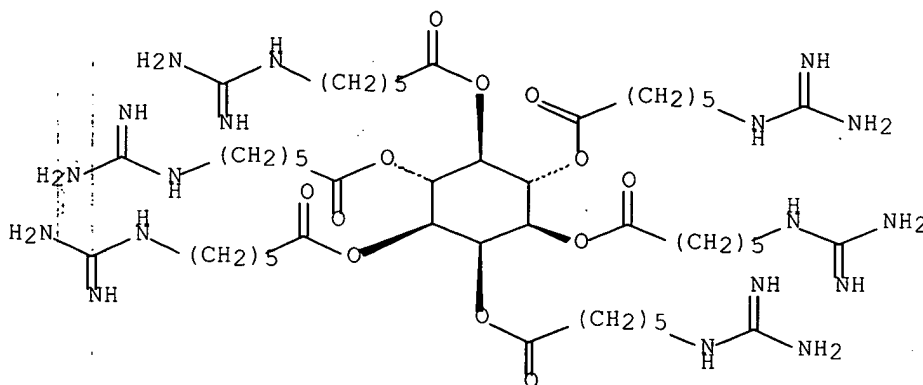
PAGE 2-A



RN 913834-25-0 HCAPLUS

CN myo-Inositol, hexakis[6-[(aminoiminomethyl)amino]hexanoate],
hexahydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



● 6 HCl

REFERENCE COUNT:

6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L148 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:923015 HCAPLUS Full-text

DOCUMENT NUMBER: 143:406069

TITLE: Divergent syntheses of all 16 carba-sugar stereoisomers via stereo-conversion of carba-β-D-altropyranose derivatives

AUTHOR(S): Yu, Seok-Ho; Chung, Sung-Kee

CORPORATE SOURCE: Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

SOURCE: Tetrahedron: Asymmetry (2005), 16(16), 2729-2747
CODEN: TASYE3; ISSN: 0957-4166

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:406069

AB We have developed practical synthetic routes to enantiopure - and -carba-β-altrose derivs. and all the possible stereoisomers via their divergent stereo-conversions. Carba-β-D-altrose was prepared from 3-cyclohexene-1-carboxylic acid and converted to carba-β-D-mannose, carba-β-D-idose, and carba-β-D-talose derivs. via regio- and stereoselective oxidation/reduction of 3-OH and/or 4-OH. The four carba-sugar stereoisomers were then transformed to the remaining 12 carba-sugar stereoisomers and their 1,2-epoxides by regio- and stereoselective manipulation of hydroxyl groups in C1 and C2, which includes oxidation/reduction, Mitsunobu's reaction, olefination/dihydroxylation, and epoxidn./ring-opening protocols.

REFERENCE COUNT: 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L148 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:708411 HCAPLUS Full-text

DOCUMENT NUMBER: 143:347371
 TITLE: Syntheses of glycodendrimers having scyllo-inositol as the scaffold
 AUTHOR(S): Lee, Nan-Young; Jang, Woo-Jae; Yu, Seok-Ho; Im, Jungkyun; Chung, Sung-Kee
 CORPORATE SOURCE: Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea
 SOURCE: Tetrahedron Letters (2005), 46(36), 6063-6066
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 143:347371

AB Synthetic glycoconjugated dendrimers have emerged as important functional glycomimetics for studying multivalency effects in the cell-cell communications. We report herein, a synthetic route to functionalized glycodendrimers with scyllo-inositol as the scaffold, which have a directed geometry; one side of the dendrimers is designed for ready attachment to the AFM probe/solid matrix, and the other to have a varying number of a sugar.

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L148 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:655924 HCAPLUS Full-text *Post Filing/Priority*
 TITLE: Practical syntheses of enantiopure carbasugars: Toward all possible 16(32) stereoisomers via divergent synthetic strategy

AUTHOR(S): Yu, Seok-Ho; Chung, Sung-Kee

CORPORATE SOURCE: Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

SOURCE: Abstracts of Papers, 228th ACS National Meeting, Philadelphia, PA, United States, August 22-26, 2004 (2004), CARB-068. American Chemical Society: Washington, D. C.

CODEN: 69FTZ8

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

AB Currently, oligosaccharides or their analogs are emerging as potential therapeutic agents. Recently we have investigated practical synthetic routes to various carbasugar stereoisomers that can be used as building blocks for non-hydrolyzable oligosaccharide analogs. As a part of our attempts to develop practical synthetic routes to all 16(32) stereoisomers of carbasugars, we have synthesized enantiopure carba- β -altrose derivs. from 3-cyclohexene-1-carboxylic acid via enzymic resolution and stereoselective introduction of hydroxyl groups at C1.apprx.C4. Furthermore regio- and stereo-selective inversions of C1.apprx.C4 of carba- β -altrose were accomplished to give carba- β -mannose, carba- β -idose, carba- β -talose, carba- α -altrose, carba- β -allose, and carba- α -allose derivs.

L148 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:106238 HCAPLUS Full-text

DOCUMENT NUMBER: 140:321600

TITLE: Practical syntheses of enantiopure carbasugars: carba- β -altrose, carba- β -mannose,

carba- β -idose, and carba- β -talose derivatives
AUTHOR(S): Yu, Seok-Ho; Chung, Sung-Kee
CORPORATE SOURCE: Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea
SOURCE: Tetrahedron: Asymmetry (2004), 15(4), 581-584
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:321600

*Doesn't teach
polymers*

AB D And L forms of carba- β -altrose, carba- β -mannose, carba- β -idose, carba- β -talose derivs. were prepared from (\pm)-3-cyclohexene-1-carboxylic acid. Homochiral diol compds., which were prepared from (\pm)-3-cyclohexene-1-carboxylic acid via enzyme resolution, were efficiently transformed to carba- β -altrose derivs. by stereoselective introduction of hydroxyl groups. Oxidation (PCC)/reduction (NaBH₄) of 3-OH and/or 4-OH of efficiently gave carba- β -mannose, carba- β -idose and carba- β -talose derivs. with good stereoselectivity.

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L148 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:316505 HCAPLUS Full-text

DOCUMENT NUMBER: 129:54509

TITLE: Syntheses of D-myo-inositol-1,2,6-trisphosphate and -2,6-bisphosphate

AUTHOR(S): Chung, Sung-Kee; Yu, Seok-Ho;
Chang, Young-Tae

No polymers

CORPORATE SOURCE: Department of Chemistry, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

SOURCE: Journal of Carbohydrate Chemistry (1998), 17(3), 385-390

CODEN: JCACDM; ISSN: 0732-8303

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 129:54509

*Doesn't teach
polymers*

AB A D-myo-inositol derivative, obtained from Me α -D-glucopyranoside by Ferrier rearrangement, was efficiently transformed to D-myo-inositol 1,2,6-trisphosphate (α -trinositol) and D-myo-inositol 2,6-bisphosphate.

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L148 ANSWER 11 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:466512 HCAPLUS Full-text

DOCUMENT NUMBER: 125:168499

TITLE: Synthesis of L-chiro-inositol-1,2,3-trisphosphate and -1,2,3,5-tetrakisphosphate by Ferrier reaction of methyl α -D-mannopyranoside

AUTHOR(S): Chung, Sung-Kee; Yu, Seok-Ho

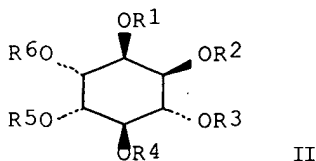
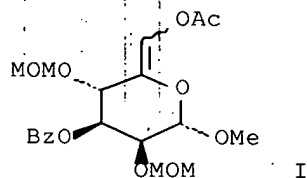
no polymers

CORPORATE SOURCE: Dep. of Chemistry, Pohang Univ. of Science & Technology, Pohang, 790-784, S. Korea

SOURCE: Bioorganic & Medicinal Chemistry Letters (1996), 6(13), 1461-1464

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB. The Ferrier rearrangement of a Me α -D-mannopyranoside derivative I, followed by a stereoselective reduction gave a L-chiro-inositol derivative II (R1 = R3 = H, R2 = Ac, R4 = R6 = MOM, R5 = Bz) which was converted to L-chiro-inositol 1,2,3-trisphosphate II (R1-R3 = PO₃H₂, R4-R6 = H) and L-chiro-inositol 1,2,3,5-tetrakisphosphate II (R1-R3 = R5 = PO₃H₂, R4 = R6 = H). These compds. may be considered to be the C3-position stereoisomers of D-myo-inositol 1,2,6-triphosphate (α -trinositol) and D-myo-inositol 1,3,4,5-tetrakisphosphate, resp., and should be useful for the binding studies with their macromol. counterparts.

L148 ANSWER 12 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:394363 HCAPLUS Full-text

DOCUMENT NUMBER: 125:114995

TITLE: Ferrier reaction of methyl α -D-mannopyranoside: synthesis of L-chiro-inositol 1,2,3-trisphosphate and 1,2,3,5-tetrakisphosphate

AUTHOR(S): Chung, Sung-Kee; Yu, Seok-Ho

CORPORATE SOURCE: Dep. Chem., Pohang Univ. Sci. Technol., Pohang, 790-784, S. Korea

SOURCE: Korean Journal of Medicinal Chemistry (1996), 6(1), 35-46

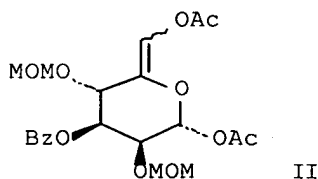
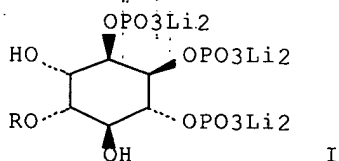
CODEN: KJMCE7; ISSN: 1225-0058

PUBLISHER: Korean Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



no polymers

AB L-Chiro-inositol phosphates I (R = H, PO₃Li₂) were prepared via Ferrier rearrangement of (Z)-mannopyranoside II followed by a stereoselective reduction. Compds. I may be considered to be the C3-position stereoisomers of D-myo-inositol 1,2,6-trisphosphate (α -trinositol) and D-myo-inositol 1,3,4,5-tetrakisphosphate, resp., and should be useful for the binding studies with their receptors and metabolic enzymes.

L148 ANSWER 13 OF 13 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:299011 HCAPLUS Full-text

DOCUMENT NUMBER: 122:187949

TITLE: Synthesis of D-6-deoxy-6,6-difluoro-myo-inositol

AUTHOR(S): Chung, Sung-Kee; Yu, Seok-Ho

CORPORATE SOURCE: Dep. Chem., Pohang Univ. Sci. Technology, Pohang, 790-784, S. Korea

SOURCE: Korean Journal of Medicinal Chemistry (1994), 4(2), 80-3

CODEN: KJMCE7; ISSN: 1225-0058

PUBLISHER: Korean Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

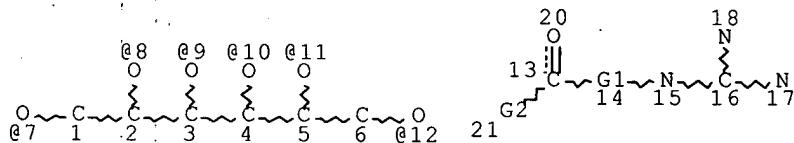
OTHER SOURCE(S): CASREACT 122:187949

AB The first synthesis of optically pure D-6-deoxy-6,6-difluoro-myo-inositol 9 was accomplished via 1-O-acetyl-2,3,4,5-tetra-O-benzyl-myo-D-inosose, the key intermediate which was prepared from Me α -D-glucopyranoside by Ferrier rearrangement.

=> => d stat que 1152

L149. STR

no polymers



REP G1=(1-12) C

VAR G2=7/8/9/10/11/12

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L151 1 5 SEA FILE=REGISTRY SSS FUL L149

L152 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L151

=> d ibib abs hitstr 1152 1-2

L152 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2007:1177686 HCAPLUS Full-text
 DOCUMENT NUMBER: 147:474696
 TITLE: Arginine prodrugs with high therapeutic activity
 INVENTOR(S): Annunziato, Lucio; Secondo, Agnese; Minale, Massimiliano; Melisi, Daniela; Rimoli, Maria Grazia; Montoro, Paola; Piacente, Sonia; De Capraris, Paolo
 PATENT ASSIGNEE(S): Farmaceutici Damor S.p.A., Italy; Universita' Degli Studi di Napoli "Federico II", Divisione di Farmacologia, Dipartimento di Neuroscienze
 SOURCE: PCT Int. Appl., 24pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007115808	A1	20071018	WO 2007-EP3145	20070406
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.:

IT 2006-MI677

A 20060406

AB: Esters of arginine (L- and/or D- enantiomers) with D-galactose useful as prodrugs are described, possessing a high capacity for penetrating cell membranes and the blood-brain barrier. The esters of the invention, once absorbed, gradually release arginine and ensure prolonged and high levels of the drug, generating a substantial and extended therapeutic response over time.

IT 952575-27-8P 952575-29-0P

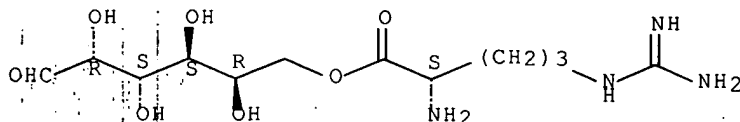
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(arginine prodrugs with high therapeutic activity)

RN 952575-27-8 HCAPLUS

CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

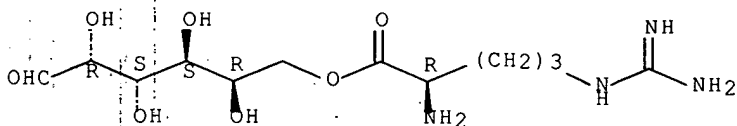


RN 952575-29-0 HCAPLUS

CN INDEX NAME NOT YET ASSIGNED

*No reason to attach to another sugar
 ↳ the arg. prodrug is the pushing is right*

Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L152 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1155705 HCAPLUS Full-text

DOCUMENT NUMBER: 145:471812

TITLE: Preparation of glycoside, oligosaccharide and cyclitol molecular transporter analogs with high permeability through biological membranes

INVENTOR(S): Chung, Sung-Kee; Maiti, Kaustabh Kumar; Lee, Woo Sirl; Jeon, Ock-Youm; Yu, Seok-Ho

PATENT ASSIGNEE(S): Postech Foundation, S. Korea; Postech Academy-Industry Foundation

SOURCE: PCT Int. Appl., 74pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

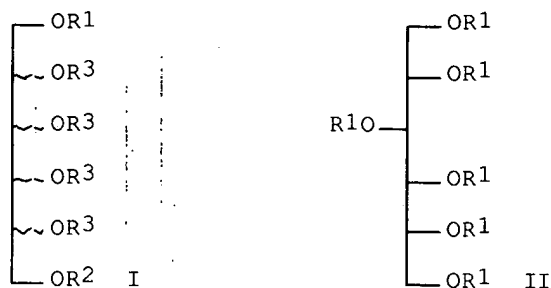
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

too late

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006/115312	A1	20061102	WO 2005-KR2040	20050629
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
KR 2006112791	A	20061102	KR 2005-35410	20050428
PRIORITY APPLN. INFO.:			KR 2005-35410	A 20050428
OTHER SOURCE(S):			MARPAT 145:471812	
GI				



AB Title compds. I, wherein R1 and R2 are independently H, alkyl, arylalkyl, cycloalkyl, etc.; R3 is a ketoalkylamino guanidine analog are prepared as mol. transporter analogs with permeability for biol. active mols. Thus, II (R1 is -CO-(CH₂)₅NH-C(=NH)-NH₂ hydrochloride salt) was prepared and tested for membrane permeability via fluorescent imaging (no data). In general, I displays good permeability when measured against an arginine nonamer for crossing biol. membrane such as a plasma membrane, nuclear membrane and blood-brain barrier.

IT 913834-21-6P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);

BIOL (Biological study); PREP (Preparation)

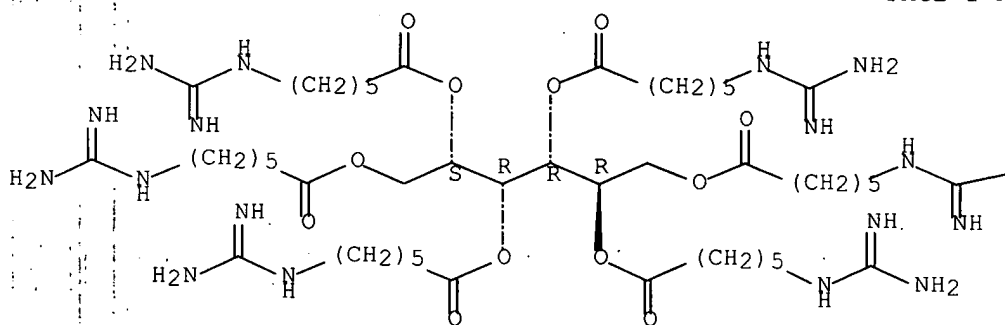
(preparation of glycoside, oligosaccharide and cyclitol mol. transporter analogs with high permeability through biol. membranes)

RN 913834-21-6 HCAPLUS

CN D-Glucitol, 1,2,3,4,5,6-hexakis[6-[(aminoiminomethyl)amino]hexanoate], hydrochloride (1:6) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



● 6 HCl

—NH₂

IT 913834-20-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

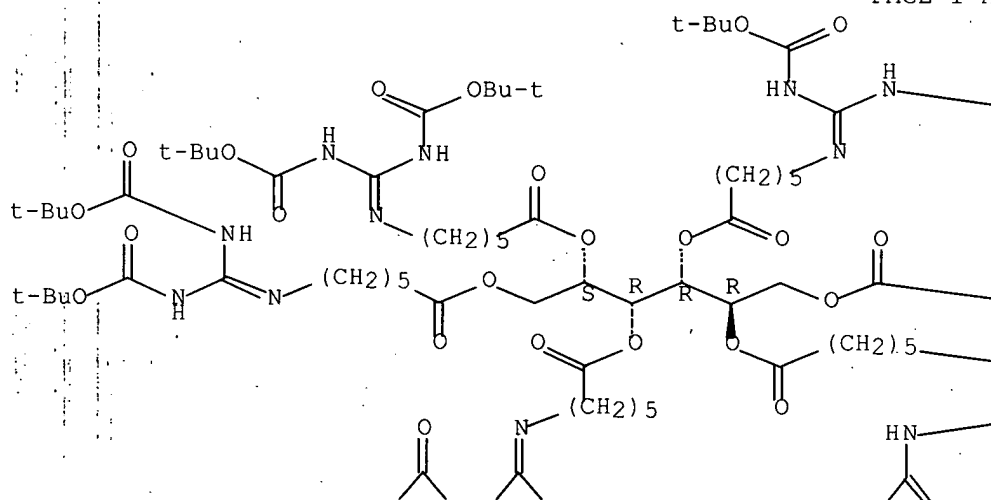
(preparation of glycoside, oligosaccharide and cyclitol mol. transporter analogs with high permeability through biol. membranes)

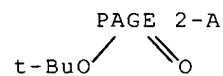
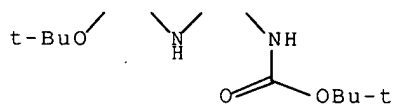
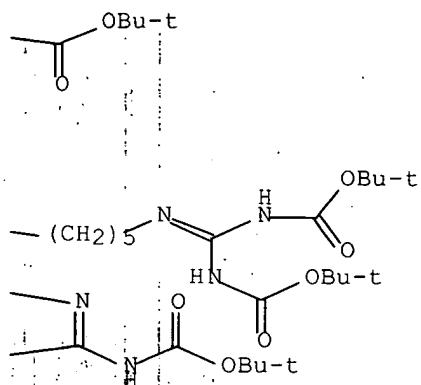
RN 913834-20-5 HCAPLUS

CN D-Glucitol, 1,2,3,4,5,6-hexakis[6-[[bis[[[(1,1-dimethylethoxy)carbonyl]amino]methylene]amino]hexanoate] (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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